TCI’s Approach to Chemical Information for Researchers
Types of Chemical Information

- Physical Properties
- Structure (SDF)
- Test / Spectral Data
- Category, Certificates, Availability, Price
- Safety & Regulatory
- Reactions, Abstracts & References
Sources of Chemical Information

- Test / Spectral Data
- Physical Properties
- Structure (SDF)
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About TCI

Worldwide Manufacturer of Chemical Reagents for Research
Provide Chemicals for the Advancement of Chemistry & All Researchers
TCI Manufacturing in Portland, OR, USA

• Collaborate with researchers and professors to prepare new compounds.
• Custom synthesize from mg to ton scale
• cGMP facilities in USA & Japan
TCI Chemicals & Product Categories

Synthetic Organic Chemistry
Bioscience
Glycoscience
Materials Chemistry
Analytical Science

...10,000 Unique Chemicals
...New Products Weekly
Examples of TCI’s Unique Chemicals

Novel Ruthenium-rhenium supramolecular photocatalyst, which is an excellent photosensitizer and can efficiently reduce CO2 to CO using solar light

[R0100] Ru-Re(FPh)

Examples of TCI’s Unique Chemicals

Cycloparaphenylenes, which are unit structures of carbon nanotubes that have attracted significant attention in recent years.

[C2931] [5]CPP

[C2449] [12]CPP

Examples of TCI’s Unique Chemicals

Pyridinium pentafluoroiiodide – hydrogenfluoride, which is a novel crystalline solid fluorinating reagent with air stability for fluorine chemistry

[Hara Reagent]

TCI - Saving Researchers Time

• Synthesize Chemicals
• Provide Chemical Reagents Quickly
• Manage & Supply Vast Amounts of Chemical Information
Choose Your Country and Language

<table>
<thead>
<tr>
<th>Americas</th>
<th>Europe</th>
<th>Asia Pacific</th>
</tr>
</thead>
<tbody>
<tr>
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<td>German</td>
<td>English</td>
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</table>
TCI America’s eShop Online Store

Campaigns
Coupons
Order History
Saved Shopping Cart
Quotation History
# TCI’s eShop - Shopping Cart

**Shopping Cart**

<table>
<thead>
<tr>
<th>Product Number</th>
<th>Product Name</th>
<th>Item Price</th>
<th>Quantity</th>
<th>Item Total</th>
<th>Your Discounted Price</th>
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Click here to update your cart with any changes you made.

**Total in Your Cart**

| Subtotal        | 463.00 USD |

We will send an order confirmation to your email address.

[Save Cart]  [Create Quotation (PDF)]  [Proceed to Checkout]
TCI Punch-Out Site

- Connect TCI’s Catalog to Procurement System
- Save Time via Automation

Multiple Languages Custom Pricing
TCI Website Features

Various Ways of Searching
Product Page : Own Dedicated Page
Links to Several Chemical Databases
Various Ways of Searching

**Simple Search** – product name, product #, or CAS #

**Structure Search** – Use JSME, ChemDraw, SMILES

**Advanced Search** – MF, MW, Category
### Specification

**Purity (GC)**: min. 95.0%

**Specific gravity (20/20)**: 0.9520 to 0.9560

**Refractive Index n20/D**: 1.3610 to 1.3650

### Data of Reference

- **bp**: 69°C (lit.)

### References

- **Reaxys-RN**: 2411211
- **PubChem SID**: 253650663

## Related Products

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<tr>
<td>T0670</td>
<td><img src="image4" alt="Structure" /></td>
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</tbody>
</table>

- TCI investigates and collects info from chemical databases (RTECS, HSDB, ICSC) and compiles with data of analysis from TCI
- SAP R/3 (SAP ERP software) & EHS-SAF to manage GHS data and physical properties

## References

- Number
- Enzyme Commission Number
- Beilstein
- Reaxys Registry Number
- PubChem Substance ID
- Merck Index Number
- Fieser & Fieser
- Registry of Toxic Effects of Chemical Substances Number
Links to the Related Academic Journals

References

Links to Several Chemical Databases

-Spectral Database for Organic Compounds SDBS
  *SDBS is owned by AIST (National Institute of Advanced Industrial Science and Technology, Japan)

-Reaxys
  *Reaxys is a trade mark of Reed Elsevier Properties SA, used under license.

-PubChem

-SciFinder
  The choice for chemistry research.

-ChemSpider
  Search and share chemistry

*Reaxys is a trade mark of Reed Elsevier Properties SA, used under license.
TCI is the only reagent manufacturer website to have a link to REAXYS.

*https://www.reaxys.com/reaxys/secure/paging.do?performed=true&action=restore

*Reaxys is a trade mark of Reed Elsevier Properties SA, used under license.
### REAXYS Link from TCI

#### Product Details

**Specification**
- **Purity (GC):** min. 95.0 %
- **Specific gravity:** 0.9520 to 0.9560
- **Refractive Index:** 1.3610 to 1.3650

**Data of Reference**
- **bp:** 99°C (lit.)

**References**
- Reaxys-RN: 2411211
- Reaxys-ID: 2478001

**Related Products**
- C1339
- H0467

### Ask TCI
Please feel free to send us your questions about our company or our products.
- 800-423-8616
- 503-283-1681

### MyTCI
MyTCI account registration allows you to use useful functions such as "My

*Reaxys is a trade mark of Reed Elsevier Properties SA, used under license.*
TCI Website Useful Links

SDBS is owned by AIST (National Institute of Advanced Industrial Science and Technology, in Japan)
SDBS is owned by AIST (National Institute of Advanced Industrial Science and Technology, in Japan)

Fact database that contains spectral patterns: Mass, NMR, IR, ESR, etc.
Download NMR Chart

4-tert-Butyl-2,6-dimethylphenylsulfur Trifluoride

Solvent : CD:CN
Internal Standard : residual Acetonitrile
Measured Temperature : 21.8°C
PubChem Link from TCI

Specification
Purity(Neutralization titration) min. 98.0 %

Data of Reference
mp 244°C(dec.)(lit.)

References
PubChem SID 87559964
ATC Index (#) 07.2
RTECS# U08925000

Related Products
T0212
M0063

PubChem SID: 87559964
PubChem CID: 2265 (azathioprine)
External ID: A2069
Source: TCI (Tokyo Chemical Industry)
Source Category: Chemical Vendors
Version: 4
Available Date: 2010.03.02
Deposit Date: 2010.03.02

Please note that the substance record below is presented as provided to PubChem by the source(depositor). For standardized chemical structure and/or the compound summary page for azathioprine.
PubChem Link to TCI

Provides chemical and physical properties, toxicity info, biological test results, etc.
SciFinder Link to TCI

Source of references, substances, and reactions in chemistry and related sciences
Reagent guides include typical reaction schemes, technical reference lists, and related product lists. Product lists categorized by applications and chemical structures.
ISSN & CODEN Assigned Journal

ISSN: 1349-4848  CODEN: TCIMCV
A New 3,3,3-trifluoropropenylolation Reagent, Ikeda–Omotani Reagent

Home > Exhibitions / Brochures Download > Quarterly Journal "TCIMAIL" > Back Numbers > A New 3,3,3-trifluoropropenylolation Reagent, Ikeda–Omotani Reagent

No.165(April 2015)

T2977 (E)-Trimethyl(3,3,3-trifluoro-1-propenyl)phosphate (1)

β-Trifluoromethylpropenyl analogues have been reported as useful compounds for liquid crystal and organic electroluminescence materials.1,2 (E)-Trimethyl(3,3,3-trifluoro-1-propenyl)phosphate (Ikeda–Omotani Reagent) (1) is a new 3,3,3-trifluoropropenylolation reagent, developed by Omotani et al. It effectively participates in a Nishiyama cross-coupling reaction with aryl iodide to construct β-trifluoromethylbenzenes in good yield.3–11 The styrene derivative provides 2-aryl-3-trifluoromethylquinolines, which may make an important contribution to drug discovery.12–14 In the presence of CuI, aryl aldehydes react with 3,3,3-trifluoropropenyl iodide in a copper-assisted cross-coupling reaction of 1 with arylacetylenes affords 1,3-disubstituted 2-fluoro-1,3-propanediols.15

Reference

TCIMAIL eNewsletter
LinkedIn
Facebook
Twitter
TCI Spares No Effort to
Move Your Chemistry Forward
and
Serve Society
through Chemical Reagents