# 1-Propene, 3-(1,1-dimethylethoxy)-

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|---|---|
| **Other names:** | Ether, allyl tert-butyl |
| | tert-Butyl Allyl ether |
| | Allyl tert-butyl ether |
| | (CH3)3COCH2CH=CH2 |
| **Inchi:** | InChI=1S/C7H14O/c1-5-6-8-7(2,3)4/h5H,1,6H2,2-4H3 |
| **InchiKey:** | FHVRTMVXBVDWCK-UHFFFAOYSA-N |
| **Formula:** | C7H14O |
| **SMILES:** | C=CCOC(C)(C)C |
| **Mol. weight [g/mol]:** | 114.19 |
| **CAS:** | 1471-04-1 |

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -6.26 | kJ/mol | Joback Method |
| hf | -203.35 | kJ/mol | Joback Method |
| hfus | 6.38 | kJ/mol | Joback Method |
| hvap | 31.62 | kJ/mol | Joback Method |
| log10ws | -1.81 | | Crippen Method |
| logp | 1.988 | | Crippen Method |
| mcvol | 111.060 | ml/mol | McGowan Method |
| pc | 2934.52 | kPa | Joback Method |
| tb | 375.43 | K | Joback Method |
| tc | 554.36 | K | Joback Method |
| tf | 191.54 | K | Joback Method |
| vc | 0.415 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 205.19 | J/mol×K | 375.43 | Joback Method |
| cpg | 217.60 | J/mol×K | 405.25 | Joback Method |
| cpg | 229.46 | J/mol×K | 435.07 | Joback Method |
| cpg | 240.78 | J/mol×K | 464.90 | Joback Method |
| cpg | 251.58 | J/mol×K | 494.72 | Joback Method |

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|---|---|---|---|---|
| cpg | 261.88 | J/mol×K | 524.54 | Joback Method |
| cpg | 271.69 | J/mol×K | 554.36 | Joback Method |
| dvisc | 0.0063127 | Pa×s | 191.54 | Joback Method |
| dvisc | 0.0025348 | Pa×s | 222.19 | Joback Method |
| dvisc | 0.0012698 | Pa×s | 252.84 | Joback Method |
| dvisc | 0.0007387 | Pa×s | 283.49 | Joback Method |
| dvisc | 0.0004776 | Pa×s | 314.13 | Joback Method |
| dvisc | 0.0003337 | Pa×s | 344.78 | Joback Method |
| dvisc | 0.0002472 | Pa×s | 375.43 | Joback Method |

# Sources

**Crippen Method:** https://www.chemeo.com/doc/models/crippen_log10ws
**Joback Method:** https://en.wikipedia.org/wiki/Joback_method
**McGowan Method:** http://link.springer.com/article/10.1007/BF02311772
**NIST Webbook:** http://webbook.nist.gov/cgi/cbook.cgi?ID=C1471041&Units=SI
**Crippen Method:** http://pubs.acs.org/doi/abs/10.1021/ci990307l

# Legend

**cpg:** Ideal gas heat capacity
**dvisc:** Dynamic viscosity
**gf:** Standard Gibbs free energy of formation
**hf:** Enthalpy of formation at standard conditions
**hfus:** Enthalpy of fusion at standard conditions
**hvap:** Enthalpy of vaporization at standard conditions
**log10ws:** Log10 of Water solubility in mol/l
**logp:** Octanol/Water partition coefficient
**mcvol:** McGowan's characteristic volume
**pc:** Critical Pressure
**tb:** Normal Boiling Point Temperature
**tc:** Critical Temperature
**tf:** Normal melting (fusion) point
**vc:** Critical Volume

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