

Glycerol, 1-tert-butyl ether

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|-----------------------------|--|
| Inchi: | InChI=1S/C7H16O3/c1-7(2,3)10-5-6(9)4-8/h6,8-9H,4-5H2,1-3H3 |
| InchiKey: | JPWDLYMEUNBLIR-UHFFFAOYSA-N |
| Formula: | C7H16O3 |
| SMILES: | CC(C)(C)OCC(O)CO |
| Mol. weight [g/mol]: | 148.20 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|----------------------|----------------|
| gf | -370.18 | kJ/mol | Joback Method |
| hf | -638.52 | kJ/mol | Joback Method |
| hfus | 12.31 | kJ/mol | Joback Method |
| hvap | 65.26 | kJ/mol | Joback Method |
| log10ws | -0.59 | | Crippen Method |
| logp | 0.155 | | Crippen Method |
| mvol | 127.100 | ml/mol | McGowan Method |
| pc | 3476.55 | kPa | Joback Method |
| rinpol | 1094.00 | | NIST Webbook |
| rinpol | 1094.00 | | NIST Webbook |
| tb | 562.67 | K | Joback Method |
| tc | 729.90 | K | Joback Method |
| tf | 299.94 | K | Joback Method |
| vc | 0.467 | m ³ /kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|-----------|---------|-----------------|---------------|
| cpg | 326.36 | J/molxK | 562.67 | Joback Method |
| cpg | 336.33 | J/molxK | 590.54 | Joback Method |
| cpg | 345.85 | J/molxK | 618.41 | Joback Method |
| cpg | 354.94 | J/molxK | 646.29 | Joback Method |
| cpg | 363.60 | J/molxK | 674.16 | Joback Method |
| cpg | 371.86 | J/molxK | 702.03 | Joback Method |
| cpg | 379.72 | J/molxK | 729.90 | Joback Method |
| dvisc | 0.0651812 | Paxs | 299.94 | Joback Method |

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|-------|-----------|------|--------|---------------|
| dvisc | 0.0084535 | Paxs | 343.73 | Joback Method |
| dvisc | 0.0017395 | Paxs | 387.52 | Joback Method |
| dvisc | 0.0004934 | Paxs | 431.30 | Joback Method |
| dvisc | 0.0001766 | Paxs | 475.09 | Joback Method |
| dvisc | 0.0000751 | Paxs | 518.88 | Joback Method |
| dvisc | 0.0000365 | Paxs | 562.67 | Joback Method |

Sources

| | |
|------------------------|---|
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=U381758&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci9903071 |
| 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 |

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 |
| rinpol: | Non-polar retention indices |
| tb: | Normal Boiling Point Temperature |
| tc: | Critical Temperature |
| tf: | Normal melting (fusion) point |
| vc: | Critical Volume |

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<https://www.chemeo.com/cid/81-125-3/Glycerol-1-tert-butyl-ether.pdf>

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