# Dipropylene glycol mono-tert-butyl ether, pentafluoropropionate

**Inchi:** InChI=1S/C13H21F5O4/c1-8(7-21-11(3,4)5)20-6-9(2)22-10(19)12(14,15)13(16,17)18/h8-

**InchiKey:** MRPIUAXKMRRSRV-UHFFFAOYSA-N

**Formula:** C13H21F5O4

**SMILES:** CC(COC(C)(C)C)OCC(C)OC(=O)C(F)(F)C(F)(F)F

**Mol. weight [g/mol]:** 336.30

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -1355.75 | kJ/mol | Joback Method |
| hf | -1838.25 | kJ/mol | Joback Method |
| hfus | 20.70 | kJ/mol | Joback Method |
| hvap | 49.76 | kJ/mol | Joback Method |
| log10ws | -3.61 | | Crippen Method |
| logp | 3.336 | | Crippen Method |
| mcvol | 222.060 | ml/mol | McGowan Method |
| pc | 1472.49 | kPa | Joback Method |
| rinpol | 1169.00 | | NIST Webbook |
| rinpol | 1169.00 | | NIST Webbook |
| tb | 603.75 | K | Joback Method |
| tc | 768.78 | K | Joback Method |
| tf | 333.10 | K | Joback Method |
| vc | 0.869 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 621.63 | J/mol×K | 603.75 | Joback Method |
| cpg | 636.97 | J/mol×K | 631.25 | Joback Method |
| cpg | 651.50 | J/mol×K | 658.76 | Joback Method |
| cpg | 665.25 | J/mol×K | 686.26 | Joback Method |
| cpg | 678.25 | J/mol×K | 713.77 | Joback Method |
| cpg | 690.52 | J/mol×K | 741.27 | Joback Method |
| cpg | 702.09 | J/mol×K | 768.78 | Joback Method |

# Sources

| | |
|---|---|
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U378342&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **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

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|---|---|
| **cpg:** | Ideal gas heat capacity |
| **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 |