# 1,3-Propanediol, O-chlorodifluoroacetate-O'-heptafluorobutyrate-

**Inchi:** InChI=1S/C9H6ClF9O4/c10-7(13,14)5(21)23-3-1-2-22-4(20)6(11,12)8(15,16)9(17,18)19/
**InchiKey:** INOCPNWOMFYNAG-UHFFFAOYSA-N
**Formula:** C9H6ClF9O4
**SMILES:** O=C(OCCCOC(=O)C(F)(F)C(F)(F)C(F)(F)F)C(F)(F)Cl
**Mol. weight [g/mol]:** 384.58

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -2196.80 | kJ/mol | Joback Method |
| hf | -2534.42 | kJ/mol | Joback Method |
| hfus | 26.90 | kJ/mol | Joback Method |
| hvap | 45.79 | kJ/mol | Joback Method |
| log10ws | -3.57 | | Crippen Method |
| logp | 3.127 | | Crippen Method |
| mcvol | 180.720 | ml/mol | McGowan Method |
| pc | 1801.56 | kPa | Joback Method |
| rinpol | 1060.00 | | NIST Webbook |
| rinpol | 1060.00 | | NIST Webbook |
| tb | 575.84 | K | Joback Method |
| tc | 733.77 | K | Joback Method |
| tf | 380.42 | K | Joback Method |
| vc | 0.754 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 482.75 | J/mol×K | 575.84 | Joback Method |
| cpg | 492.49 | J/mol×K | 602.16 | Joback Method |
| cpg | 501.55 | J/mol×K | 628.48 | Joback Method |
| cpg | 509.96 | J/mol×K | 654.81 | Joback Method |
| cpg | 517.76 | J/mol×K | 681.13 | Joback Method |
| cpg | 524.99 | J/mol×K | 707.45 | Joback Method |
| cpg | 531.67 | J/mol×K | 733.77 | 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=U375557&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |

# Legend

| | |
|---|---|
| **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 |