# Hexatriacontyl pentafluoropropionate

**Other names:** Hexatriacontyl 2,2,3,3,3-pentafluoropropanoate
1-Hexatriacontanol, pentafluoropropionate
**Inchi:** InChI=1S/C39H73F5O2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-23
**InchiKey:** LOCRWHYJIWHMIX-UHFFFAOYSA-N
**Formula:** C39H73F5O2
**SMILES:** CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCOC(=O)C(F)(F)C(F)(F)F
**Mol. weight [g/mol]:** 668.99

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -924.79 | kJ/mol | Joback Method |
| hf | -2091.14 | kJ/mol | Joback Method |
| hfus | 100.12 | kJ/mol | Joback Method |
| hvap | 104.89 | kJ/mol | Joback Method |
| log10ws | -15.99 | | Crippen Method |
| logp | 15.011 | | Crippen Method |
| mcvol | 576.660 | ml/mol | McGowan Method |
| pc | 384.02 | kPa | Joback Method |
| rinpol | 3742.40 | | NIST Webbook |
| tb | 1157.90 | K | Joback Method |
| tc | 1616.18 | K | Joback Method |
| tf | 609.24 | K | Joback Method |
| vc | 2.312 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 2191.68 | J/mol×K | 1157.90 | Joback Method |
| cpg | 2238.27 | J/mol×K | 1234.28 | Joback Method |
| cpg | 2281.17 | J/mol×K | 1310.66 | Joback Method |
| cpg | 2321.86 | J/mol×K | 1387.04 | Joback Method |
| cpg | 2361.86 | J/mol×K | 1463.42 | Joback Method |
| cpg | 2402.66 | J/mol×K | 1539.80 | Joback Method |
| cpg | 2445.76 | J/mol×K | 1616.18 | Joback Method |

# Sources

| | |
|---|---|
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U351890&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

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