# Heptafluorobutyric acid, hexadecyl ester

**Other names:** Hexadecyl heptafluorobutanoate
Hexadecyl heptafluorobutyrate
1-Hexadecanol, HFB
**Inchi:** InChI=1S/C20H33F7O2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-29-17(28)18(21,22)19
**InchiKey:** HXCITEKMLXXCSM-UHFFFAOYSA-N
**Formula:** C20H33F7O2
**SMILES:** CCCCCCCCCCCCCCCCOC(=O)C(F)(F)C(F)(F)C(F)(F)F
**Mol. weight [g/mol]:** 438.46
**CAS:** 6385-15-5

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -1471.55 | kJ/mol | Joback Method |
| hf | -2099.95 | kJ/mol | Joback Method |
| hfus | 49.66 | kJ/mol | Joback Method |
| hvap | 59.66 | kJ/mol | Joback Method |
| log10ws | -8.35 | | Crippen Method |
| logp | 7.844 | | Crippen Method |
| mcvol | 312.490 | ml/mol | McGowan Method |
| pc | 891.07 | kPa | Joback Method |
| rinpol | 1847.20 | | NIST Webbook |
| rinpol | 1847.20 | | NIST Webbook |
| rinpol | 1862.00 | | NIST Webbook |
| rinpol | 1845.00 | | NIST Webbook |
| ripol | 1891.00 | | NIST Webbook |
| ripol | 1891.00 | | NIST Webbook |
| tb | 718.49 | K | Joback Method |
| tc | 880.76 | K | Joback Method |
| tf | 398.71 | K | Joback Method |
| vc | 1.272 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|

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|---|---|---|---|---|
| cpg | 966.88 | J/mol×K | 718.49 | Joback Method |
| cpg | 984.56 | J/mol×K | 745.53 | Joback Method |
| cpg | 1001.32 | J/mol×K | 772.58 | Joback Method |
| cpg | 1017.20 | J/mol×K | 799.62 | Joback Method |
| cpg | 1032.26 | J/mol×K | 826.67 | Joback Method |
| cpg | 1046.55 | J/mol×K | 853.71 | Joback Method |
| cpg | 1060.12 | J/mol×K | 880.76 | Joback Method |

# Sources

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|---|---|
| **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=C6385155&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |

# 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 |
| **ripol:** | Polar retention indices |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |