# Heptafluorobutyric acid, 3-methyl ester

**Inchi:** InChI=1S/C11H7F7O2/c1-6-3-2-4-7(5-6)20-8(19)9(12,13)10(14,15)11(16,17)18/h2-5H,1H
**InchiKey:** NTTFSSUNLZOBKZ-UHFFFAOYSA-N
**Formula:** C11H7F7O2
**SMILES:** Cc1cccc(OC(=O)C(F)(F)C(F)(F)C(F)(F)F)c1
**Mol. weight [g/mol]:** 304.16

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -1444.55 | kJ/mol | Joback Method |
| hf | -1689.13 | kJ/mol | Joback Method |
| hfus | 20.00 | kJ/mol | Joback Method |
| hvap | 42.57 | kJ/mol | Joback Method |
| log10ws | -4.39 | | Crippen Method |
| logp | 3.733 | | Crippen Method |
| mcvol | 161.920 | ml/mol | McGowan Method |
| pc | 2123.64 | kPa | Joback Method |
| tb | 544.23 | K | Joback Method |
| tc | 723.63 | K | Joback Method |
| tf | 336.22 | K | Joback Method |
| vc | 0.660 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 413.92 | J/mol×K | 544.23 | Joback Method |
| cpg | 426.16 | J/mol×K | 574.13 | Joback Method |
| cpg | 437.49 | J/mol×K | 604.03 | Joback Method |
| cpg | 447.97 | J/mol×K | 633.93 | Joback Method |
| cpg | 457.66 | J/mol×K | 663.83 | Joback Method |
| cpg | 466.59 | J/mol×K | 693.73 | Joback Method |
| cpg | 474.82 | J/mol×K | 723.63 | Joback Method |

# Sources

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|---|---|
| **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 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U307627&Units=SI |

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