# Fumaric acid, naphth-1-yl 2,2,3,3,4,4,5,5-octafluoropentyl ester

**Inchi:** InChI=1S/C19H12F8O4/c20-16(21)18(24,25)19(26,27)17(22,23)10-30-14(28)8-9-15(29)3

**InchiKey:** LLEZEWRGGFVBDU-CMDGGOBGSA-N

**Formula:** C19H12F8O4

**SMILES:** O=C(C=CC(=O)Oc1cccc2ccccc12)OCC(F)(F)C(F)(F)C(F)(F)C(F)F

**Mol. weight [g/mol]:** 456.28

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -1621.49 | kJ/mol | Joback Method |
| hf | -1992.15 | kJ/mol | Joback Method |
| hfus | 40.29 | kJ/mol | Joback Method |
| hvap | 69.92 | kJ/mol | Joback Method |
| log10ws | -6.49 | | Crippen Method |
| logp | 5.016 | | Crippen Method |
| mcvol | 260.090 | ml/mol | McGowan Method |
| pc | 1443.54 | kPa | Joback Method |
| rinpol | 2258.00 | | NIST Webbook |
| rinpol | 2258.00 | | NIST Webbook |
| tb | 825.53 | K | Joback Method |
| tc | 1023.88 | K | Joback Method |
| tf | 511.75 | K | Joback Method |
| vc | 1.046 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 783.81 | J/mol×K | 825.53 | Joback Method |
| cpg | 794.60 | J/mol×K | 858.59 | Joback Method |
| cpg | 804.60 | J/mol×K | 891.65 | Joback Method |
| cpg | 813.92 | J/mol×K | 924.70 | Joback Method |
| cpg | 822.67 | J/mol×K | 957.76 | Joback Method |
| cpg | 830.94 | J/mol×K | 990.82 | Joback Method |
| cpg | 838.85 | J/mol×K | 1023.88 | Joback Method |

# Sources

| | |
|---|---|
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U405804&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 |

# 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 |