# 1-Naphthoic acid, 2,2,3,3,4,4,5,5-octafluoropentyl ester

**Inchi:** InChI=1S/C16H10F8O2/c17-13(18)15(21,22)16(23,24)14(19,20)8-26-12(25)11-7-3-5-9-4

**InchiKey:** LFTALLNVWKRZAG-UHFFFAOYSA-N

**Formula:** C16H10F8O2

**SMILES:** O=C(OCC(F)(F)C(F)(F)C(F)(F)C(F)F)c1cccc2ccccc12

**Mol. weight [g/mol]:** 386.24

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -1493.05 | kJ/mol | Joback Method |
| hf | -1802.65 | kJ/mol | Joback Method |
| hfus | 29.53 | kJ/mol | Joback Method |
| hvap | 54.13 | kJ/mol | Joback Method |
| log10ws | -6.45 | | Crippen Method |
| logp | 5.168 | | Crippen Method |
| mcvol | 214.680 | ml/mol | McGowan Method |
| pc | 1676.91 | kPa | Joback Method |
| rinpol | 1837.00 | | NIST Webbook |
| tb | 676.44 | K | Joback Method |
| tc | 863.64 | K | Joback Method |
| tf | 410.86 | K | Joback Method |
| vc | 0.875 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 609.81 | J/mol×K | 676.44 | Joback Method |
| cpg | 622.09 | J/mol×K | 707.64 | Joback Method |
| cpg | 633.41 | J/mol×K | 738.84 | Joback Method |
| cpg | 643.84 | J/mol×K | 770.04 | Joback Method |
| cpg | 653.47 | J/mol×K | 801.24 | Joback Method |
| cpg | 662.38 | J/mol×K | 832.44 | Joback Method |
| cpg | 670.66 | J/mol×K | 863.64 | Joback Method |

# Sources

| | |
|---|---|
| **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=U355684&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 |
| **rinpol:** | Non-polar retention indices |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |