# Adipic acid, decyl 2,2,3,3,4,4,5,5-octafluoropentyl ester

**Inchi:** InChI=1S/C21H32F8O4/c1-2-3-4-5-6-7-8-11-14-32-16(30)12-9-10-13-17(31)33-15-19(24

**InchiKey:** MHLDTAZGCARVKW-UHFFFAOYSA-N

**Formula:** C21H32F8O4

**SMILES:** CCCCCCCCCCOC(=O)CCCCC(=O)OCC(F)(F)C(F)(F)C(F)(F)C(F)F

**Mol. weight [g/mol]:** 500.46

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -1894.30 | kJ/mol | Joback Method |
| hf | -2566.78 | kJ/mol | Joback Method |
| hfus | 54.59 | kJ/mol | Joback Method |
| hvap | 69.84 | kJ/mol | Joback Method |
| log10ws | -7.59 | | Crippen Method |
| logp | 6.945 | | Crippen Method |
| mcvol | 335.790 | ml/mol | McGowan Method |
| pc | 846.53 | kPa | Joback Method |
| rinpol | 2211.00 | | NIST Webbook |
| rinpol | 2211.00 | | NIST Webbook |
| tb | 816.49 | K | Joback Method |
| tc | 1000.80 | K | Joback Method |
| tf | 467.73 | K | Joback Method |
| vc | 1.365 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 1092.24 | J/mol×K | 816.49 | Joback Method |
| cpg | 1109.25 | J/mol×K | 847.21 | Joback Method |
| cpg | 1125.20 | J/mol×K | 877.93 | Joback Method |
| cpg | 1140.14 | J/mol×K | 908.64 | Joback Method |
| cpg | 1154.15 | J/mol×K | 939.36 | Joback Method |
| cpg | 1167.28 | J/mol×K | 970.08 | Joback Method |
| cpg | 1179.59 | J/mol×K | 1000.80 | Joback Method |

# Sources

| | |
|---|---|
| **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=U353736&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |

# 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 |