# Sebacic acid, 3,5-difluorophenyl octyl ester

**Inchi:** InChI=1S/C24H36F2O4/c1-2-3-4-5-10-13-16-29-23(27)14-11-8-6-7-9-12-15-24(28)30-22
**InchiKey:** LIBHTAMKVAMZQG-UHFFFAOYSA-N
**Formula:** C24H36F2O4
**SMILES:** CCCCCCCCOC(=O)CCCCCCCCC(=O)Oc1cc(F)cc(F)c1
**Mol. weight [g/mol]:** 426.54

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -613.11 | kJ/mol | Joback Method |
| hf | -1206.92 | kJ/mol | Joback Method |
| hfus | 62.91 | kJ/mol | Joback Method |
| hvap | 89.30 | kJ/mol | Joback Method |
| log10ws | -8.01 | | Crippen Method |
| logp | 6.895 | | Crippen Method |
| mcvol | 343.680 | ml/mol | McGowan Method |
| pc | 965.07 | kPa | Joback Method |
| rinpol | 2845.00 | | NIST Webbook |
| rinpol | 2845.00 | | NIST Webbook |
| tb | 936.28 | K | Joback Method |
| tc | 1146.56 | K | Joback Method |
| tf | 557.20 | K | Joback Method |
| vc | 1.355 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 1132.84 | J/mol×K | 936.28 | Joback Method |
| cpg | 1149.49 | J/mol×K | 971.33 | Joback Method |
| cpg | 1164.76 | J/mol×K | 1006.37 | Joback Method |
| cpg | 1178.68 | J/mol×K | 1041.42 | Joback Method |
| cpg | 1191.29 | J/mol×K | 1076.47 | Joback Method |
| cpg | 1202.62 | J/mol×K | 1111.51 | Joback Method |
| cpg | 1212.71 | J/mol×K | 1146.56 | Joback Method |

# Sources

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|---|---|
| **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=U354530&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 |