# Diethylmalonic acid, 2-fluoroethyl tridecyl ester

**Inchi:** InChI=1S/C22H41FO4/c1-4-7-8-9-10-11-12-13-14-15-16-18-26-20(24)22(5-2,6-3)21(25)2

**InchiKey:** IMLQSXHGGGBCNR-UHFFFAOYSA-N

**Formula:** C22H41FO4

**SMILES:** CCCCCCCCCCCCCOC(=O)C(CC)(CC)C(=O)OCCF

**Mol. weight [g/mol]:** 388.56

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -525.45 | kJ/mol | Joback Method |
| hf | -1191.87 | kJ/mol | Joback Method |
| hfus | 53.98 | kJ/mol | Joback Method |
| hvap | 80.77 | kJ/mol | Joback Method |
| log10ws | -6.37 | | Crippen Method |
| logp | 6.160 | | Crippen Method |
| mcvol | 337.490 | ml/mol | McGowan Method |
| pc | 938.64 | kPa | Joback Method |
| rinpol | 2361.00 | | NIST Webbook |
| tb | 851.38 | K | Joback Method |
| tc | 1042.47 | K | Joback Method |
| tf | 485.03 | K | Joback Method |
| vc | 1.323 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 1099.80 | J/mol×K | 851.38 | Joback Method |
| cpg | 1118.60 | J/mol×K | 883.23 | Joback Method |
| cpg | 1136.24 | J/mol×K | 915.08 | Joback Method |
| cpg | 1152.76 | J/mol×K | 946.92 | Joback Method |
| cpg | 1168.19 | J/mol×K | 978.77 | Joback Method |
| cpg | 1182.59 | J/mol×K | 1010.62 | Joback Method |
| cpg | 1195.99 | J/mol×K | 1042.47 | 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=U370867&Units=SI |

# 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 |