# Glutaric acid, 1-(2,6-difluorophenyl)ethyl hexadecyl ester

**Inchi:** InChI=1S/C29H46F2O4/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-16-23-34-27(32)21-18-22-2

**InchiKey:** UUPBAIDEASSMDB-UHFFFAOYSA-N

**Formula:** C29H46F2O4

**SMILES:** CCCCCCCCCCCCCCCCOC(=O)CCCC(=O)OC(C)c1c(F)cccc1F

**Mol. weight [g/mol]:** 496.67

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -573.45 | kJ/mol | Joback Method |
| hf | -1315.40 | kJ/mol | Joback Method |
| hfus | 72.34 | kJ/mol | Joback Method |
| hvap | 100.04 | kJ/mol | Joback Method |
| log10ws | -9.91 | | Crippen Method |
| logp | 8.764 | | Crippen Method |
| mcvol | 414.130 | ml/mol | McGowan Method |
| pc | 734.03 | kPa | Joback Method |
| rinpol | 3306.00 | | NIST Webbook |
| tb | 1050.24 | K | Joback Method |
| tc | 1302.25 | K | Joback Method |
| tf | 598.55 | K | Joback Method |
| vc | 1.629 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 1445.63 | J/mol×K | 1050.24 | Joback Method |
| cpg | 1464.17 | J/mol×K | 1092.24 | Joback Method |
| cpg | 1480.60 | J/mol×K | 1134.24 | Joback Method |
| cpg | 1495.01 | J/mol×K | 1176.24 | Joback Method |
| cpg | 1507.49 | J/mol×K | 1218.24 | Joback Method |
| cpg | 1518.13 | J/mol×K | 1260.24 | Joback Method |
| cpg | 1527.00 | J/mol×K | 1302.25 | 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=U377261&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 |

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