

Glutaric acid, 3,4-difluorobenzyl undecyl ester

Inchi: InChI=1S/C23H34F2O4/c1-2-3-4-5-6-7-8-9-10-16-28-22(26)12-11-13-23(27)29-18-19-14
InchiKey: GNWHURVHYAREAM-UHFFFAOYSA-N
Formula: C23H34F2O4
SMILES: CCCCCCCCCCOC(=O)CCCC(=O)OCc1ccc(F)c(F)c1
Mol. weight [g/mol]: 412.51

Physical Properties

| Property code | Value | Unit | Source |
|---------------|----------|----------------------|----------------|
| gf | -621.53 | kJ/mol | Joback Method |
| hf | -1186.28 | kJ/mol | Joback Method |
| hfus | 60.32 | kJ/mol | Joback Method |
| hvap | 87.07 | kJ/mol | Joback Method |
| log10ws | -7.44 | | Crippen Method |
| logp | 6.252 | | Crippen Method |
| mvol | 329.590 | ml/mol | McGowan Method |
| pc | 1025.31 | kPa | Joback Method |
| rinpol | 3025.00 | | NIST Webbook |
| rinpol | 3025.00 | | NIST Webbook |
| tb | 913.40 | K | Joback Method |
| tc | 1118.29 | K | Joback Method |
| tf | 545.93 | K | Joback Method |
| vc | 1.300 | m ³ /kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|---------|---------|-----------------|---------------|
| cpg | 1071.65 | J/molxK | 913.40 | Joback Method |
| cpg | 1087.95 | J/molxK | 947.55 | Joback Method |
| cpg | 1102.97 | J/molxK | 981.70 | Joback Method |
| cpg | 1116.72 | J/molxK | 1015.84 | Joback Method |
| cpg | 1129.25 | J/molxK | 1049.99 | Joback Method |
| cpg | 1140.57 | J/molxK | 1084.14 | Joback Method |
| cpg | 1150.73 | J/molxK | 1118.29 | Joback Method |

Sources

| | |
|------------------------|---|
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci9903071 |
| 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=U377642&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 |
| rinpola: | Non-polar retention indices |
| tb: | Normal Boiling Point Temperature |
| tc: | Critical Temperature |
| tf: | Normal melting (fusion) point |
| vc: | Critical Volume |

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