

Glutaric acid, decyl 3,4-difluorobenzyl ester

| | |
|-----------------------------|--|
| Inchi: | InChI=1S/C22H32F2O4/c1-2-3-4-5-6-7-8-9-15-27-21(25)11-10-12-22(26)28-17-18-13-14 |
| InchiKey: | MAGJLWSQENYJEJ-UHFFFAOYSA-N |
| Formula: | C22H32F2O4 |
| SMILES: | CCCCCCCCCOC(=O)CCCC(=O)OCc1ccc(F)c(F)c1 |
| Mol. weight [g/mol]: | 398.48 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|----------|----------------------|----------------|
| gf | -629.95 | kJ/mol | Joback Method |
| hf | -1165.64 | kJ/mol | Joback Method |
| hfus | 57.73 | kJ/mol | Joback Method |
| hvap | 84.84 | kJ/mol | Joback Method |
| log10ws | -7.02 | | Crippen Method |
| logp | 5.862 | | Crippen Method |
| mvol | 315.500 | ml/mol | McGowan Method |
| pc | 1091.38 | kPa | Joback Method |
| rinpol | 2917.00 | | NIST Webbook |
| rinpol | 2917.00 | | NIST Webbook |
| tb | 890.52 | K | Joback Method |
| tc | 1090.98 | K | Joback Method |
| tf | 534.66 | K | Joback Method |
| vc | 1.244 | m ³ /kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|---------|---------|-----------------|---------------|
| cpg | 1011.05 | J/mol×K | 890.52 | Joback Method |
| cpg | 1027.01 | J/mol×K | 923.93 | Joback Method |
| cpg | 1041.77 | J/mol×K | 957.34 | Joback Method |
| cpg | 1055.35 | J/mol×K | 990.75 | Joback Method |
| cpg | 1067.77 | J/mol×K | 1024.16 | Joback Method |
| cpg | 1079.07 | J/mol×K | 1057.57 | Joback Method |
| cpg | 1089.26 | J/mol×K | 1090.98 | Joback Method |

Sources

| | |
|------------------------|---|
| 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=U377641&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| Crippen Method: | https://www.cheméo.com/doc/models/crippen_log10ws |

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 |

Latest version available from:

<https://www.cheméo.com/cid/116-297-4/Glutaric-acid-decyl-3-4-difluorobenzyl-ester.pdf>

Generated by Cheméo on 2026-03-11 07:30:13.864294358 +0000 UTC m=+3611905.557363604.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.