

Terephthalic acid, 2-fluoro-6-(trifluoromethyl)benzyl nonyl ester

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| Inchi: | InChI=1S/C25H28F4O4/c1-2-3-4-5-6-7-8-16-32-23(30)18-12-14-19(15-13-18)24(31)33-1 |
| InchiKey: | IJEAEWXFRVNDC-UHFFFAOYSA-N |
| Formula: | C25H28F4O4 |
| SMILES: | CCCCCCCCOC(=O)c1ccc(C(=O)OCc2c(F)cccc2C(F)(F)F)cc1 |
| Mol. weight [g/mol]: | 468.48 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|----------|----------------------|----------------|
| gf | -888.69 | kJ/mol | Joback Method |
| hf | -1403.47 | kJ/mol | Joback Method |
| hfus | 57.90 | kJ/mol | Joback Method |
| hvap | 91.53 | kJ/mol | Joback Method |
| log10ws | -8.85 | | Crippen Method |
| logp | 7.109 | | Crippen Method |
| mvol | 337.550 | ml/mol | McGowan Method |
| pc | 1061.02 | kPa | Joback Method |
| rinpol | 3308.00 | | NIST Webbook |
| rinpol | 3308.00 | | NIST Webbook |
| tb | 986.13 | K | Joback Method |
| tc | 1207.41 | K | Joback Method |
| tf | 611.01 | K | Joback Method |
| vc | 1.329 | m ³ /kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|---------|---------|-----------------|---------------|
| cpg | 1102.50 | J/molxK | 986.13 | Joback Method |
| cpg | 1115.97 | J/molxK | 1023.01 | Joback Method |
| cpg | 1128.17 | J/molxK | 1059.89 | Joback Method |
| cpg | 1139.15 | J/molxK | 1096.77 | Joback Method |
| cpg | 1148.98 | J/molxK | 1133.65 | Joback Method |
| cpg | 1157.74 | J/molxK | 1170.53 | Joback Method |
| cpg | 1165.48 | J/molxK | 1207.41 | Joback Method |

Sources

| | |
|------------------------|---|
| 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=U382950&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci990307I |

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 |
| hvp: | 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 |
| rinp: | Non-polar retention indices |
| tb: | Normal Boiling Point Temperature |
| tc: | Critical Temperature |
| tf: | Normal melting (fusion) point |
| vc: | Critical Volume |

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