# Phthalic acid, decyl 3-fluorobenzyl ester

**Inchi:** InChI=1S/C25H31FO4/c1-2-3-4-5-6-7-8-11-17-29-24(27)22-15-9-10-16-23(22)25(28)30-1
**InchiKey:** XAIZCEQRRYICHN-UHFFFAOYSA-N
**Formula:** C25H31FO4
**SMILES:** CCCCCCCCCCOC(=O)c1ccccc1C(=O)OCc1cccc(F)c1
**Mol. weight [g/mol]:** 414.51

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -297.47 | kJ/mol | Joback Method |
| hf | -794.92 | kJ/mol | Joback Method |
| hfus | 56.46 | kJ/mol | Joback Method |
| hvap | 94.61 | kJ/mol | Joback Method |
| log10ws | -8.17 | | Crippen Method |
| logp | 6.480 | | Crippen Method |
| mcvol | 332.240 | ml/mol | McGowan Method |
| pc | 1157.71 | kPa | Joback Method |
| rinpol | 2951.00 | | NIST Webbook |
| tb | 986.57 | K | Joback Method |
| tc | 1209.75 | K | Joback Method |
| tf | 594.30 | K | Joback Method |
| vc | 1.286 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 1082.82 | J/mol×K | 986.57 | Joback Method |
| cpg | 1096.93 | J/mol×K | 1023.77 | Joback Method |
| cpg | 1109.61 | J/mol×K | 1060.96 | Joback Method |
| cpg | 1120.93 | J/mol×K | 1098.16 | Joback Method |
| cpg | 1130.93 | J/mol×K | 1135.35 | Joback Method |
| cpg | 1139.66 | J/mol×K | 1172.55 | Joback Method |
| cpg | 1147.18 | J/mol×K | 1209.75 | Joback Method |

# Sources

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|---|---|
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U377894&Units=SI |
| **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 |

# Legend

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|---|---|
| **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 |