# Diglycolic acid, 2-chloro-6-fluorophenyl isohexyl ester

**Inchi:** InChI=1S/C16H20ClFO5/c1-11(2)5-4-8-22-14(19)9-21-10-15(20)23-16-12(17)6-3-7-13(1
**InchiKey:** UFFHXJOUVHZDAK-UHFFFAOYSA-N
**Formula:** C16H20ClFO5
**SMILES:** CC(C)CCCOC(=O)COCC(=O)Oc1c(F)cccc1Cl
**Mol. weight [g/mol]:** 346.78

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -605.03 | kJ/mol | Joback Method |
| hf | -998.93 | kJ/mol | Joback Method |
| hfus | 40.97 | kJ/mol | Joback Method |
| hvap | 78.71 | kJ/mol | Joback Method |
| log10ws | -3.86 | | Crippen Method |
| logp | 3.380 | | Crippen Method |
| mcvol | 247.300 | ml/mol | McGowan Method |
| pc | 1663.26 | kPa | Joback Method |
| rinpol | 2717.00 | | NIST Webbook |
| rinpol | 2717.00 | | NIST Webbook |
| tb | 813.38 | K | Joback Method |
| tc | 1016.16 | K | Joback Method |
| tf | 503.60 | K | Joback Method |
| vc | 0.951 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 709.51 | J/mol×K | 813.38 | Joback Method |
| cpg | 722.71 | J/mol×K | 847.18 | Joback Method |
| cpg | 734.89 | J/mol×K | 880.97 | Joback Method |
| cpg | 746.04 | J/mol×K | 914.77 | Joback Method |
| cpg | 756.17 | J/mol×K | 948.56 | Joback Method |
| cpg | 765.26 | J/mol×K | 982.36 | Joback Method |
| cpg | 773.32 | J/mol×K | 1016.16 | Joback Method |

# Sources

| | |
|---|---|
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U381943&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 |
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |

# 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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