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

**Inchi:** InChI=1S/C19H26ClFO5/c1-2-3-4-5-6-7-8-12-25-17(22)13-24-14-18(23)26-19-15(20)10-9

**InchiKey:** HFKQIFMVKMPXNE-UHFFFAOYSA-N

**Formula:** C19H26ClFO5

**SMILES:** CCCCCCCCCOC(=O)COCC(=O)Oc1c(F)cccc1Cl

**Mol. weight [g/mol]:** 388.86

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -577.33 | kJ/mol | Joback Method |
| hf | -1055.57 | kJ/mol | Joback Method |
| hfus | 52.27 | kJ/mol | Joback Method |
| hvap | 85.78 | kJ/mol | Joback Method |
| log10ws | -5.36 | | Crippen Method |
| logp | 4.695 | | Crippen Method |
| mcvol | 289.570 | ml/mol | McGowan Method |
| pc | 1324.24 | kPa | Joback Method |
| rinpol | 3272.00 | | NIST Webbook |
| rinpol | 3272.00 | | NIST Webbook |
| tb | 882.46 | K | Joback Method |
| tc | 1085.81 | K | Joback Method |
| tf | 552.41 | K | Joback Method |
| vc | 1.125 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 880.91 | J/mol×K | 882.46 | Joback Method |
| cpg | 894.73 | J/mol×K | 916.35 | Joback Method |
| cpg | 907.38 | J/mol×K | 950.24 | Joback Method |
| cpg | 918.86 | J/mol×K | 984.13 | Joback Method |
| cpg | 929.17 | J/mol×K | 1018.02 | Joback Method |
| cpg | 938.33 | J/mol×K | 1051.92 | Joback Method |
| cpg | 946.33 | J/mol×K | 1085.81 | 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=U381947&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

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