# Fumaric acid, monoamide, N-(5-chloro-2-methoxyphenyl)-, 2-pentyl ester

**Inchi:** InChI=1S/C16H20ClNO4/c1-4-5-11(2)22-16(20)9-8-15(19)18-13-10-12(17)6-7-14(13)21-

**InchiKey:** XWDWFFOSEUQCGF-CMDGGOBGSA-N

**Formula:** C16H20ClNO4

**SMILES:** CCCC(C)OC(=O)C=CC(=O)Nc1cc(Cl)ccc1OC

**Mol. weight [g/mol]:** 325.79

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -135.61 | kJ/mol | Joback Method |
| hf | -499.91 | kJ/mol | Joback Method |
| hfus | 42.01 | kJ/mol | Joback Method |
| hvap | 83.51 | kJ/mol | Joback Method |
| log10ws | -4.24 | | Crippen Method |
| logp | 3.575 | | Crippen Method |
| mcvol | 245.340 | ml/mol | McGowan Method |
| pc | 1849.92 | kPa | Joback Method |
| rinpol | 2718.00 | | NIST Webbook |
| tb | 846.02 | K | Joback Method |
| tc | 1062.40 | K | Joback Method |
| tf | 528.36 | K | Joback Method |
| vc | 0.929 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 702.56 | J/mol×K | 846.02 | Joback Method |
| cpg | 715.39 | J/mol×K | 882.08 | Joback Method |
| cpg | 727.19 | J/mol×K | 918.15 | Joback Method |
| cpg | 738.00 | J/mol×K | 954.21 | Joback Method |
| cpg | 747.84 | J/mol×K | 990.27 | Joback Method |
| cpg | 756.74 | J/mol×K | 1026.34 | Joback Method |
| cpg | 764.72 | J/mol×K | 1062.40 | 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=U357498&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |

# 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 |