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

**Inchi:** InChI=1S/C16H20ClNO4/c1-16(2,3)10-22-15(20)8-7-14(19)18-12-9-11(17)5-6-13(12)21-4

**InchiKey:** AWQMGJDVYVKQHQ-BQYQJAHWSA-N

**Formula:** C16H20ClNO4

**SMILES:** COc1ccc(Cl)cc1NC(=O)C=CC(=O)OCC(C)(C)C

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

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -130.33 | kJ/mol | Joback Method |
| hf | -503.38 | kJ/mol | Joback Method |
| hfus | 38.12 | kJ/mol | Joback Method |
| hvap | 82.60 | kJ/mol | Joback Method |
| log10ws | -3.88 | | Crippen Method |
| logp | 3.433 | | Crippen Method |
| mcvol | 245.340 | ml/mol | McGowan Method |
| pc | 1867.55 | kPa | Joback Method |
| rinpol | 2680.00 | | NIST Webbook |
| rinpol | 2680.00 | | NIST Webbook |
| tb | 843.23 | K | Joback Method |
| tc | 1064.73 | K | Joback Method |
| tf | 545.78 | K | Joback Method |
| vc | 0.924 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 703.38 | J/mol×K | 843.23 | Joback Method |
| cpg | 716.23 | J/mol×K | 880.15 | Joback Method |
| cpg | 728.08 | J/mol×K | 917.06 | Joback Method |
| cpg | 738.96 | J/mol×K | 953.98 | Joback Method |
| cpg | 748.94 | J/mol×K | 990.89 | Joback Method |
| cpg | 758.05 | J/mol×K | 1027.81 | Joback Method |
| cpg | 766.35 | J/mol×K | 1064.73 | Joback Method |

# Sources

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|---|---|
| **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 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U357517&Units=SI |

# 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 |