# Benzamide, 2,4,5-trifluoro-3-methoxy-N-octyl-

**Inchi:** InChI=1S/C16H22F3NO2/c1-3-4-5-6-7-8-9-20-16(21)11-10-12(17)14(19)15(22-2)13(11)1
**InchiKey:** BIIYMFJZPDYYMU-UHFFFAOYSA-N
**Formula:** C16H22F3NO2
**SMILES:** CCCCCCCCNC(=O)c1cc(F)c(F)c(OC)c1F
**Mol. weight [g/mol]:** 317.35

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -571.23 | kJ/mol | Joback Method |
| hf | -962.58 | kJ/mol | Joback Method |
| hfus | 46.81 | kJ/mol | Joback Method |
| hvap | 69.28 | kJ/mol | Joback Method |
| log10ws | -5.86 | | Crippen Method |
| logp | 4.203 | | Crippen Method |
| mcvol | 235.270 | ml/mol | McGowan Method |
| pc | 1527.07 | kPa | Joback Method |
| rinpol | 2141.00 | | NIST Webbook |
| rinpol | 2141.00 | | NIST Webbook |
| tb | 736.35 | K | Joback Method |
| tc | 918.99 | K | Joback Method |
| tf | 473.17 | K | Joback Method |
| vc | 0.936 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 679.42 | J/mol×K | 736.35 | Joback Method |
| cpg | 693.89 | J/mol×K | 766.79 | Joback Method |
| cpg | 707.57 | J/mol×K | 797.23 | Joback Method |
| cpg | 720.49 | J/mol×K | 827.67 | Joback Method |
| cpg | 732.65 | J/mol×K | 858.11 | Joback Method |
| cpg | 744.07 | J/mol×K | 888.55 | Joback Method |
| cpg | 754.76 | J/mol×K | 918.99 | Joback Method |

# Sources

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|---|---|
| **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=U407645&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |

# 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 |