# Sarcosine, n-(4-fluorobenzoyl)-, isohexyl ester

**Inchi:** InChI=1S/C16H22FNO3/c1-12(2)5-4-10-21-15(19)11-18(3)16(20)13-6-8-14(17)9-7-13/h6
**InchiKey:** HJOAOINBZKWCBD-UHFFFAOYSA-N
**Formula:** C16H22FNO3
**SMILES:** CC(C)CCCOC(=O)CN(C)C(=O)c1ccc(F)cc1
**Mol. weight [g/mol]:** 295.35

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| hfus | 37.81 | kJ/mol | Joback Method |
| logp | 2.877 | | Crippen Method |
| mcvol | 233.300 | ml/mol | McGowan Method |
| rinpol | 2126.00 | | NIST Webbook |
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## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 669.25 | J/mol×K | 738.57 | Joback Method |
| cpg | 684.49 | J/mol×K | 771.44 | Joback Method |
| cpg | 698.76 | J/mol×K | 804.31 | Joback Method |
| cpg | 712.09 | J/mol×K | 837.18 | Joback Method |
| cpg | 724.52 | J/mol×K | 870.05 | Joback Method |
| cpg | 736.07 | J/mol×K | 902.92 | Joback Method |
| cpg | 746.78 | J/mol×K | 935.79 | Joback Method |

## Sources

**Joback Method:** https://en.wikipedia.org/wiki/Joback_method
**McGowan Method:** http://link.springer.com/article/10.1007/BF02311772
**Crippen Method:** http://pubs.acs.org/doi/abs/10.1021/ci990307l
**Crippen Method:** https://www.chemeo.com/doc/models/crippen_log10ws

**Cheméo Relay (1.0):**

**Cheméo Relay (1.0, beta):**

**NIST Webbook:** http://webbook.nist.gov/cgi/cbook.cgi?ID=U321310&Units=SI

# Legend

| | |
|---|---|
| **cpg:** | Ideal gas heat capacity |
| **hfus:** | Enthalpy of fusion at standard conditions |
| **logp:** | Octanol/Water partition coefficient |
| **mcvol:** | McGowan's characteristic volume |
| **rinpol:** | Non-polar retention indices |