

Isobutylcarbamate, N-(4-methylphenyl)

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|-----------------------------|--|
| Inchi: | InChI=1S/C12H17NO2/c1-9(2)8-15-12(14)13-11-6-4-10(3)5-7-11/h4-7,9H,8H2,1-3H3,(H, |
| InchiKey: | ZLLWSPYPMXWEGF-UHFFFAOYSA-N |
| Formula: | C12H17NO2 |
| SMILES: | Cc1ccc(NC(=O)OCC(C)C)cc1 |
| Mol. weight [g/mol]: | 207.27 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|----------------------|----------------|
| gf | 5.97 | kJ/mol | Joback Method |
| hf | -262.56 | kJ/mol | Joback Method |
| hfus | 24.85 | kJ/mol | Joback Method |
| hvap | 60.45 | kJ/mol | Joback Method |
| log10ws | -3.23 | | Crippen Method |
| logp | 3.200 | | Crippen Method |
| mcvol | 173.600 | ml/mol | McGowan Method |
| pc | 2532.82 | kPa | Joback Method |
| rinpola | 1700.00 | | NIST Webbook |
| rinpola | 1700.00 | | NIST Webbook |
| tb | 631.64 | K | Joback Method |
| tc | 842.61 | K | Joback Method |
| tf | 373.76 | K | Joback Method |
| vc | 0.652 | m ³ /kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|--------|---------|-----------------|---------------|
| cpg | 445.86 | J/molxK | 631.64 | Joback Method |
| cpg | 460.85 | J/molxK | 666.80 | Joback Method |
| cpg | 474.96 | J/molxK | 701.96 | Joback Method |
| cpg | 488.20 | J/molxK | 737.13 | Joback Method |
| cpg | 500.60 | J/molxK | 772.29 | Joback Method |
| cpg | 512.17 | J/molxK | 807.45 | Joback Method |
| cpg | 522.93 | J/molxK | 842.61 | Joback Method |

Sources

| | |
|------------------------|---|
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci9903071 |
| Crippen Method: | https://www.cheméo.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=R392533&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 |
| hvp: | 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 |
| rinp: | Non-polar retention indices |
| tb: | Normal Boiling Point Temperature |
| tc: | Critical Temperature |
| tf: | Normal melting (fusion) point |
| vc: | Critical Volume |

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