

N,N-Dimethyl-N'-(4-methoxyphenyl)-isobutyramid

Inchi: InChI=1S/C13H20N2O/c1-10(2)13(15(3)4)14-11-6-8-12(16-5)9-7-11/h6-10H,1-5H3
InchiKey: CGVIDZOLZWHOFX-UHFFFAOYSA-N
Formula: C13H20N2O
SMILES: COc1ccc(N=C(C(C)C)N(C)C)cc1
Mol. weight [g/mol]: 220.31

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| hf | -84.13 | kJ/mol | Joback Method |
| hvap | 54.93 | kJ/mol | Joback Method |
| log10ws | -2.66 | | Crippen Method |
| logp | 2.943 | | Crippen Method |
| mcvol | 191.800 | ml/mol | McGowan Method |
| pc | 1956.14 | kPa | Joback Method |
| rinpol | 1769.00 | | NIST Webbook |
| tb | 639.48 | K | Joback Method |
| tc | 855.52 | K | Joback Method |

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R162535&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
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>

Legend

hf: Enthalpy of formation 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 |

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