

N,N-Dimethyl-2-phenyl-N'-(3-nitrophenyl)-acetami

Inchi: InChI=1S/C16H17N3O2/c1-18(2)16(11-13-7-4-3-5-8-13)17-14-9-6-10-15(12-14)19(20)21
InchiKey: VEWXQPHGXDPFKW-WUKNDPDISA-N
Formula: C16H17N3O2
SMILES: CN(C)C(Cc1ccccc1)=Nc1cccc([N+](=O)[O-])c1
Mol. weight [g/mol]: 283.33

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| hf | 217.22 | kJ/mol | Joback Method |
| hvap | 78.45 | kJ/mol | Joback Method |
| log10ws | -4.21 | | Crippen Method |
| logp | 3.429 | | Crippen Method |
| mcvol | 221.860 | ml/mol | McGowan Method |
| pc | 2071.76 | kPa | Joback Method |
| rinpol | 2511.00 | | NIST Webbook |
| tb | 864.66 | K | Joback Method |
| tc | 1125.85 | K | Joback Method |

Sources

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>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R162179&Units=SI>

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 |

Latest version available from:

<https://www.cheméo.com/cid/43-295-7/N-N-Dimethyl-2-phenyl-N-3-nitrophenyl-acetamide.pdf>

Generated by Cheméo on 2024-04-26 04:04:21.745071259 +0000 UTC m=+16393510.665648571.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.