

N'-(4-fluoro-phenyl)-N,N-dimethyl-acetamide

Inchi: InChI=1S/C10H13FN2/c1-8(13(2)3)12-10-6-4-9(11)5-7-10/h4-7H,1-3H3/b12-8+
InchiKey: FBMSXVILQYIGIO-XYOKQWHBSA-N
Formula: C10H13FN2
SMILES: CC(=Nc1ccc(F)cc1)N(C)C
Mol. weight [g/mol]: 180.22

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| hf | -80.82 | kJ/mol | Joback Method |
| hvap | 45.41 | kJ/mol | Joback Method |
| log10ws | -2.27 | | Crippen Method |
| logp | 2.437 | | Crippen Method |
| mcvol | 145.430 | ml/mol | McGowan Method |
| pc | 2477.65 | kPa | Joback Method |
| rinpol | 1465.00 | | NIST Webbook |
| tb | 548.13 | K | Joback Method |
| tc | 762.92 | K | Joback Method |

Sources

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=R153407&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307I>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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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