

p-chlorobenzylidene-cyclohexyl-amine

Inchi: InChI=1S/C13H16ClN/c14-12-8-6-11(7-9-12)10-15-13-4-2-1-3-5-13/h6-10,13H,1-5H2/b14
InchiKey: JAXKXTHEYAPNGE-XNTDXEJSSA-N
Formula: C13H16ClN
SMILES: Clc1ccc(C=NC2CCCCC2)cc1
Mol. weight [g/mol]: 221.73

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| hf | 34.21 | kJ/mol | Joback Method |
| hvap | 55.60 | kJ/mol | Joback Method |
| log10ws | -4.32 | | Crippen Method |
| logp | 4.092 | | Crippen Method |
| mcvol | 177.330 | ml/mol | McGowan Method |
| pc | 2295.91 | kPa | Joback Method |
| rinpol | 1872.00 | | NIST Webbook |
| rinpol | 1872.00 | | NIST Webbook |
| tb | 662.16 | K | Joback Method |
| tc | 918.77 | 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=R159876&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 |

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