

2-Phenethylamine, N-dimethylaminomethylene-

Inchi: InChI=1S/C11H16N2/c1-13(2)10-12-9-8-11-6-4-3-5-7-11/h3-7,10H,8-9H2,1-2H3
InchiKey: KPDUVWBTRFPCGC-UHFFFAOYSA-N
Formula: C11H16N2
SMILES: CN(C)C=NCCc1ccccc1
Mol. weight [g/mol]: 176.26

Physical Properties

Property code	Value	Unit	Source
hf	115.91	kJ/mol	Joback Method
hvap	47.71	kJ/mol	Joback Method
log10ws	-1.76		Crippen Method
logp	1.819		Crippen Method
mcvol	157.750	ml/mol	McGowan Method
pc	2379.54	kPa	Joback Method
rinpol	1449.00		NIST Webbook
rinpol	1449.00		NIST Webbook
tb	566.88	K	Joback Method
tc	783.82	K	Joback Method

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U376190&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307I>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method: https://en.wikipedia.org/wiki/Joback_method

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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