

N-Phenethylazetidine

Inchi:	InChI=1S/C11H15N/c1-2-5-11(6-3-1)7-10-12-8-4-9-12/h1-3,5-6H,4,7-10H2
InchiKey:	VIXGVWUHTYYAH-UHFFFAOYSA-N
Formula:	C11H15N
SMILES:	c1ccc(CCN2CCC2)cc1
Mol. weight [g/mol]:	161.24
CAS:	42525-65-5

Physical Properties

Property code	Value	Unit	Source
chl	-6594.00 ± 1.30	kJ/mol	NIST Webbook
hf	185.20 ± 2.10	kJ/mol	NIST Webbook
hfl	122.00 ± 1.30	kJ/mol	NIST Webbook
hvap	63.20	kJ/mol	NIST Webbook
log10ws	-1.99		Crippen Method
logp	1.935		Crippen Method
mcpvol	141.210	ml/mol	McGowan Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hvapt	62.20	kJ/mol	317.50	NIST Webbook
hvapt	63.20 ± 0.92	kJ/mol	303.00	NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C42525655&Units=SI

Legend

chl:	Standard liquid enthalpy of combustion
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase enthalpy of formation at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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