Dibenz[b,e]azepin, 5,6(11H)dihydro-

Other names: 11H-Dibenz[b,E]azepine, 5,6-dihydro-
6,11-dihydro-5H-dibenz[b,e]azepine
Dibenz[b,e]azepin, 5,6(11H)dihydro-
Inchi: InChI=1S/C14H13N/c1-2-7-13-10-15-14-8-4-3-6-12(14)9-11(13)5-1/h1-8,15H,9-10H2
InchiKey: YSHVGIKWUJCBLY-UHFFFAOYSA-N
Formula: C14H13N
SMILES: c1ccc2c(c1)CNc1ccccc1C2
Mol. weight [g/mol]: 195.27

Physical Properties

Property code	Value	Unit	Source
hf	247.65	kJ/mol	Cheméo Relay (1.0)
hfus	25.97	kJ/mol	Joback Method
hvap	92.50	kJ/mol	Cheméo Relay (1.0)
ie	7.34	eV	Cheméo Relay (1.0)
log10ws	-3.84		Cheméo Relay (1.0)
logp	3.203		Crippen Method
mcvol	159.720	ml/mol	McGowan Method
tb	631.54	K	Cheméo Relay (1.0)
tc	909.36	K	Cheméo Relay (1.0)
tf	401.73	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	399.28	J/mol×K	643.00	Joback Method
cpg	416.02	J/mol×K	686.76	Joback Method
cpg	431.36	J/mol×K	730.51	Joback Method
cpg	445.45	J/mol×K	774.27	Joback Method
cpg	458.39	J/mol×K	818.03	Joback Method
cpg	470.32	J/mol×K	861.78	Joback Method
cpg	481.36	J/mol×K	905.54	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C449558&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point

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