

5H-Dibenz[b,e]azepine, 6,11-dihydro-

Other names:	Dibenz[b,e]azepin, 5,6(11H)dihydro-11H-Dibenz[b,E]azepine, 5,6-dihydro-6,11-dihydro-5H-dibenz[b,e]azepine
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:	YSHVGIKWUJCPLY-UHFFFAOYSA-N
Formula:	C14H13N
SMILES:	<chem>c1ccc2c(c1)CNc1cccc1C2</chem>
Mol. weight [g/mol]:	195.26
CAS:	449-55-8

Physical Properties

Property code	Value	Unit	Source
gf	428.73	kJ/mol	Joback Method
hf	248.78	kJ/mol	Joback Method
hfus	25.97	kJ/mol	Joback Method
hvap	59.61	kJ/mol	Joback Method
log10ws	-3.94		Crippen Method
logp	3.203		Crippen Method
mcvol	159.720	ml/mol	McGowan Method
pc	3295.37	kPa	Joback Method
tb	643.00	K	Joback Method
tc	905.54	K	Joback Method
tf	452.63	K	Joback Method
vc	0.599	m3/kmol	Joback Method

Temperature Dependent Properties

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

Sources

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

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion 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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

Latest version available from:

<https://www.cheméo.com/cid/78-522-6/5H-Dibenz-b-e-azepine-6-11-dihydro.pdf>

Generated by Cheméo on 2024-04-28 19:41:45.290253462 +0000 UTC m=+16622554.210830777.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.