5H-Dibenz[b,f]azepine, 10,11-dihydro-

Other names:	10,11-Dihydro-5-dibenz(b,f)azepine 10,11-Dihydro-5H-dibenz[b,f]azepine 10,11-dihydro-5H-dibenzo[b,f]azepine 10,11-dihydrodibenz[b,f]azepine 2,2'-Iminobibenzyl 2,2'-iminodibenzyl 5H-Dibenzo[b,f]azepine, 10,11-dihydro- Iminodibenzyyl NSC 72110 RP 23669 iminobibenzyl iminodibenzyl
Inchi:	InChI=1S/C14H13N/c1-3-7-13-11(5-1)9-10-12-6-2-4-8-14(12)15-13/h1-8,15H,9-10H2
InchiKey:	ZSMRRZONCYIFNB-UHFFFAOYSA-N
Formula:	C14H13N
SMILES:	c1ccc2c(c1)CCc1ccccc1N2
Mol. weight [g/mol]:	195.26
CAS:	494-19-9

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
ie	7.25	eV	NIST Webbook
log10ws	-3.94		Crippen Method
logp	3.529		Crippen Method
mcvol	159.720	ml/mol	McGowan Method
pc	3295.37	kPa	Joback Method
rinpol	1931.00		NIST Webbook
rinpol	1980.00		NIST Webbook
rinpol	1931.00		NIST Webbook
rinpol	1931.00		NIST Webbook
rinpol	1931.00		NIST Webbook
rinpol	1931.00		NIST Webbook
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/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

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Equilibrium solubility determination, modelling and preferential solvation of bioactive mimosdibenzyl in aqueous co-solvent mixtures at various temperatures:	https://www.doi.org/10.1016/j.jct.2018.12.045
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=C494199&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
ie:	Ionization energy
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
tf:	Normal melting (fusion) point
vc:	Critical Volume