Iminostilbene

Other names:	5H-Dibenz[b,f]azepine
	Dibenz(b,f)azepine
	Stilbene, 2,2'-imino-
	2,2'-Iminostilbene
	2,3,6,7-Dibenzazepine
	5-Azadibenzo(a,e)cycloheptatriene
	5H-Dibenzo(b,f)azepine
	NSC 123458
	o,o'-Iminostilbene
Inchi:	InChI=1S/C14H11N/c1-3-7-13-11(5-1)9-10-12-6-2-4-8-14(12)15-13/h1-10,15H
InchiKey:	LCGTWRLJTMHIQZ-UHFFFAOYSA-N
Formula:	C14H11N
SMILES:	C1=Cc2ccccc2Nc2ccccc21
Mol. weight [g/mol]:	193.24
CAS:	256-96-2

Physical Properties

Property code	Value	Unit	Source
gf	458.69	kJ/mol	Joback Method
hf	306.56	kJ/mol	Joback Method
hfus	27.20	kJ/mol	Joback Method
hvap	59.91	kJ/mol	Joback Method
ie	6.78	eV	NIST Webbook
log10ws	-4.13		Crippen Method
logp	3.914		Crippen Method
mcvol	155.420	ml/mol	McGowan Method
pc	3435.91	kPa	Joback Method
rinpol	2021.00		NIST Webbook
rinpol	2021.00		NIST Webbook
rinpol	1985.00		NIST Webbook
rinpol	1985.00		NIST Webbook
tb	642.16	K	Joback Method
tc	907.38	K	Joback Method
tf	453.39	K	Joback Method
vc	0.585	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	377.12	J/mol×K	642.16	Joback Method
cpg	392.57	J/mol×K	686.36	Joback Method
cpg	406.68	J/mol×K	730.57	Joback Method
cpg	419.58	J/mol×K	774.77	Joback Method
cpg	431.41	J/mol×K	818.97	Joback Method
cpg	442.30	J/mol×K	863.18	Joback Method
cpg	452.38	J/mol×K	907.38	Joback Method

Sources

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=C256962&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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