

Benzenamine, N-(phenylmethylene)-, N-oxide

Other names:	Benzaldehydephenylnitron Nitron, N,«alpha»-diphenyl- «alpha»,N-Diphenylnitron C,N-Diphenylnitron Diphenylnitron N,«alpha»-Diphenylnitron N-benzylideneaniline N-oxide
Inchi:	InChI=1S/C13H11NO/c15-14(13-9-5-2-6-10-13)11-12-7-3-1-4-8-12/h1-11H
InchiKey:	ZEAUJQWDPKRESH-UHFFFAOYSA-N
Formula:	C13H11NO
SMILES:	[O-][N+](=Cc1ccccc1)c1ccccc1
Mol. weight [g/mol]:	197.23
CAS:	1137-96-8

Physical Properties

Property code	Value	Unit	Source
chs	-6835.70 ± 1.00	kJ/mol	NIST Webbook
hf	263.00 ± 2.10	kJ/mol	NIST Webbook
hfs	148.00 ± 2.00	kJ/mol	NIST Webbook
hsub	115.00 ± 0.80	kJ/mol	NIST Webbook
hsub	115.00 ± 0.80	kJ/mol	NIST Webbook
log10ws	-3.23		Crippen Method
logp	2.947		Crippen Method
mcvol	158.060	ml/mol	McGowan Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C1137968&Units=SI

Legend

chs:	Standard solid enthalpy of combustion
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation at standard conditions
hsub:	Enthalpy of sublimation at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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