

Phenol, 2-[(phenylimino)methyl]-, N-oxide

Other names:	Nitrone, «alpha»-(o-hydroxyphenyl)-N-phenyl- «alpha»-(o-Hydroxyphenyl)-N-phenylnitrone Nitrone, «alpha»-(2-hydroxyphenyl)-N-phenyl-
Inchi:	InChI=1S/C13H11NO2/c15-13-9-5-4-6-11(13)10-14(16)12-7-2-1-3-8-12/h1-10,15H
InchiKey:	ORXOGPXBVINWDG-UHFFFAOYSA-N
Formula:	C13H11NO2
SMILES:	[O-][N+](=Cc1ccccc1O)c1ccccc1
Mol. weight [g/mol]:	213.23
CAS:	20357-59-9

Physical Properties

Property code	Value	Unit	Source
chs	-6625.10 ± 1.10	kJ/mol	NIST Webbook
hf	53.90 ± 2.40	kJ/mol	NIST Webbook
hfs	-62.60 ± 2.00	kJ/mol	NIST Webbook
hsub	116.50 ± 1.40	kJ/mol	NIST Webbook
hsub	116.50 ± 1.40	kJ/mol	NIST Webbook
log10ws	-2.78		Crippen Method
logp	2.653		Crippen Method
mcvol	163.930	ml/mol	McGowan Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C20357599&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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