Phenol, 2-(2-benzothiazolyl)-

Other names:	2-(2'-Hydroxyphenyl)benzothiazole
	2-(2-Benzothiazolyl)phenol
	2-(2-hydroxyphenyl)-1,3-benzothiazole
	2-(2-hydroxyphenyl)benzothiazole
	2-(benzo[d]thiazol-2-yl)phenol
	2-(o-Hydroxyphenyl)benzothiazole
	2-benzothiazol-2-ylphenol
	NSC 5051
	NSC 58548
	Phenol, o-2-benzothiazolyl-
	o-(2-Benzothiazolyl)phenol
	o-(2-Benzothiazoyl)phenol
Inchi:	InChI=1S/C13H9NOS/c15-11-7-3-1-5-9(11)13-14-10-6-2-4-8-12(10)16-13/h1-8,15H
InchiKey:	MVVGSPCXHRFDDR-UHFFFAOYSA-N
Formula:	C13H9NOS
SMILES:	Oc1ccccc1-c1nc2ccccc2s1
Mol. weight [g/mol]:	227.28
CAS:	3411-95-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.95		Crippen Method
logp	3.669		Crippen Method
mcvol	163.550	ml/mol	McGowan Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hvapt	105.00	kJ/mol	298.15	Thermochemical and conformational study of optical active phenylbenzazole derivatives

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3411958&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Thermochemical and conformational study of optical active phenylbenzazole derivatives:	https://www.doi.org/10.1016/j.jct.2017.08.017

Legend

hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume