

Phenol, 2-(2-benzoxazolyl)-

Other names:	Phenol, o-2-benzoxazolyl- 2-(o-Hydroxyphenyl)benzoxazole 2-(2-Hydroxyphenyl)benzoxazole 2-(ortho-Hydroxyphenyl)-benzoxazole o-(2-Benzoxazolyl)phenol 2-(O-Hydroxyphenyl)benzoxazol USAF EK-6754 2-(1,3-Benzoxazol-2-yl)phenol NSC 403545 NSC 5423 2-benzoxazol-2-ylphenol
Inchi:	InChI=1S/C13H9NO2/c15-11-7-3-1-5-9(11)13-14-10-6-2-4-8-12(10)16-13/h1-8,15H
InchiKey:	GHGZVWOTJDLREY-UHFFFAOYSA-N
Formula:	C13H9NO2
SMILES:	Oc1cccc1-c1nc2cccc2o1
Mol. weight [g/mol]:	211.22
CAS:	835-64-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.93		Crippen Method
logp	3.200		Crippen Method
mcvol	153.070	ml/mol	McGowan Method
tb	611.20	K	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C835643&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature

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