

2(3H)-Benzoxazolone

Other names:	2-Benzoxazolinone Carbamic acid, (2-hydroxyphenyl)-, «gamma»-lactone 2-Benzoxazolol 2-Benzoxazolone Benzoxazolone Benzoxazole, 2-hydroxy- Benzoxazolinone USAF EK-5429 2-Hydroxybenzoxazole NSC 3812
Inchi:	InChI=1S/C7H5NO2/c9-7-8-5-3-1-2-4-6(5)10-7/h1-4H,(H,8,9)
InchiKey:	ASSKVPFEZFFQQNQ-UHFFFAOYSA-N
Formula:	C7H5NO2
SMILES:	O=c1[nH]c2ccccc2o1
Mol. weight [g/mol]:	135.12
CAS:	59-49-4

Physical Properties

Property code	Value	Unit	Source
hsub	97.60 ± 2.20	kJ/mol	NIST Webbook
log10ws	-5.65		Crippen Method
logp	0.639		Crippen Method
mcvol	92.290	ml/mol	McGowan Method
tf	410.65 ± 1.50	K	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C59494&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

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
tf:	Normal melting (fusion) point

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