2(3H)-Benzoxazolone, 6-chloro-

Other names:	2-Benzoxazolinone, 6-chloro-
	6-Chloro-2-benzoxazolinone
	6-Chloro-2-benzoxazolone
	6-Chlorobenzoxazolinone
	6-Chlorobenzoxazolone
	HOE 54014
Inchi:	InChI=1S/C7H4ClNO2/c8-4-1-2-5-6(3-4)11-7(10)9-5/h1-3H,(H,9,10)
InchiKey:	MATCZHXABVLZIE-UHFFFAOYSA-N
Formula:	C7H4ClNO2
SMILES:	O=c1[nH]c2ccc(Cl)cc2o1
Mol. weight [g/mol]:	169.56
CAS:	19932-84-4

Physical Properties

Property code	Value	Unit	Source
chs	-3002.80 ± 3.50	kJ/mol	NIST Webbook
hfs	-346.70 ± 3.90	kJ/mol	NIST Webbook
log10ws	-6.34		Crippen Method
logp	1.293		Crippen Method
mcvol	104.530	ml/mol	McGowan Method

Sources

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=C19932844&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

chs:	Standard solid enthalpy of combustion

hfs:	Solid phase enthalpy of formation at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume