

Benzoxazole, 2-chloro-

Other names:	2-Chlorobenzoxazole
Inchi:	InChI=1S/C7H4ClNO/c8-7-9-5-3-1-2-4-6(5)10-7/h1-4H
InchiKey:	BBVQDWDBTWSGHQ-UHFFFAOYSA-N
Formula:	C7H4ClNO
SMILES:	Clc1nc2ccccc2o1
Mol. weight [g/mol]:	153.57
CAS:	615-18-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.46		Crippen Method
logp	2.481		Crippen Method
mvol	98.660	ml/mol	McGowan Method
tb	474.70	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hvapt	56.30	kJ/mol	298.15	Experimental and computational thermochemical studies of benzoxazole and two chlorobenzoxadole derivatives

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C615189&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Experimental and computational thermochemical studies of benzoxazole and two chlorobenzoxadole derivatives:	https://www.doi.org/10.1016/j.jct.2012.08.028

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
tb:	Normal Boiling Point Temperature

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