

Benzothiazole, 2-chloro-

Other names:	2-Chlorobenzothiazole USAF ek-2784
Inchi:	InChI=1S/C7H4CINS/c8-7-9-5-3-1-2-4-6(5)10-7/h1-4H
InchiKey:	BSQLQMLFTHJVKS-UHFFFAOYSA-N
Formula:	C7H4CINS
SMILES:	Clc1nc2ccccc2s1
Mol. weight [g/mol]:	169.63
CAS:	615-20-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.48		Crippen Method
logp	2.950		Crippen Method
mcpol	109.140	ml/mol	McGowan Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	414.20	K	4.00	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C615203&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

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tbrp:	Boiling point at reduced pressure

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