

Thiazole, 2-bromo-

Other names:	2-Bromo-1,3-thiazole 2-Bromothiazole
Inchi:	InChI=1S/C3H2BrNS/c4-3-5-1-2-6-3/h1-2H
InchiKey:	RXNZFHIEDZEUQM-UHFFFAOYSA-N
Formula:	C3H2BrNS
SMILES:	Brc1nccs1
Mol. weight [g/mol]:	164.02
CAS:	3034-53-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.16		Crippen Method
logp	1.906		Crippen Method
mcvol	77.500	ml/mol	McGowan Method
tb	444.20	K	NIST Webbook
tb	444.00	K	NIST Webbook

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=C3034535&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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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