

6-Nitrobenzothiazole

Other names:	Benzothiazole, 6-nitro-
Inchi:	InChI=1S/C7H4N2O2S/c10-9(11)5-1-2-6-7(3-5)12-4-8-6/h1-4H
InchiKey:	QLUFBCVWKTWKBKBF-UHFFFAOYSA-N
Formula:	C7H4N2O2S
SMILES:	O=[N+](O-)c1ccc2ncsc2c1
Mol. weight [g/mol]:	180.18
CAS:	2942-06-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.45		Crippen Method
logp	2.204		Crippen Method
mcvol	114.320	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2942065&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

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