

2(3H)-Benzothiazolethione, 6-nitro-

Other names:	2-Benzothiazolinethione, 6-nitro- 2-Mercapto-6-nitrobenzothiazole 6-Nitro-2-mercaptobenzothiazole 6-Nitrobenzothiazole-2-thiol USAF EK-3991 2-Benzothiazolethiol, 6-nitro- Benzothiazole-2-thiol, 6-nitro- Benzothiazole, 2-mercapto-6-nitro- 6-Nitro-1,3-benzothiazole-2-thiol NSC 2630
Inchi:	InChI=1S/C7H4N2O2S2/c10-9(11)4-1-2-5-6(3-4)13-7(12)8-5/h1-3H,(H,8,12)
InchiKey:	QPOZGXKWWKLJDK-UHFFFAOYSA-N
Formula:	C7H4N2O2S2
SMILES:	O=[N+](O-)c1ccc2nc(S)sc2c1
Mol. weight [g/mol]:	212.25
CAS:	4845-58-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.96		Crippen Method
logp	2.493		Crippen Method
mvol	130.670	ml/mol	McGowan Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4845583&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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