2,1,3-Benzothiadiazole, 4-nitro-

Other names:	4-nitro-1,2,3-benzothiadiazole
	4-nitro-2,1,3-benzothiadiazole
	4-nitropiazthiole
Inchi:	InChI=1S/C6H3N3O2S/c10-9(11)5-3-1-2-4-6(5)8-12-7-4/h1-3H
InchiKey:	IWQKAMJGVIHECB-UHFFFAOYSA-N
Formula:	C6H3N3O2S
SMILES:	O=[N+]([O-])c1cccc2nsnc12
Mol. weight [g/mol]:	181.17
CAS:	6583-06-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.22		Crippen Method
logp	1.599		Crippen Method
mcvol	110.210	ml/mol	McGowan Method
tf	383.00	K	Energetic and structural properties of 4-nitro-2,1,3-benzothiadiazole

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Energetic and structural properties of 4-nitro-2,1,3-benzothiadiazole:	https://www.doi.org/10.1016/j.jct.2012.01.018
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6583068&Units=SI

Legend

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

tf: Normal melting (fusion) point