2-Benzothiazolesulfenamide, N-(1,1-dimethylethyl)-

Other names: 2-(tert-Butylaminothio)benzothiazole
2-Benzothiazolesulfenamide, N-tert-butyl-
Accel BNS
Akrochem BBTS
BBTS
Benzothiazolesulfenamide, N-(1,1-dimethylethyl)-
Benzothiazolyl-2-tert-butylsulfenamide
Butyl 2-benzothiazole sulfenamide
Delac NS
N-t-Butyl-2-benzothiazole-sulfenamide
N-t-Butyl-2-benzothioazole sulfenamide
N-t-Butyl-O-benzothiazole-2-sulfenamide
N-tert-Butyl-2-benzothiazolesulfenamid
N-tert-Butyl-2-benzothiazolesulfenamide
N-tert-Butyl-2-benzothiazolesulphenamide
N-tert-Butyl-2-benzothiazolylsulfenamide
N-tert-Butyl-2-benzothiazylsulfenamide
N-tert-butylbenzothiazole-2-sulphenamide
NSC 84176
NTBBTS
Nocceler NS
Pennac TBBS
Perkacit TBBS
S-(benzo[d]thiazol-2-yl)-N-(tert-butyl)thiohydroxylamine
Santocure NS
Santocure TBBS
TBBS
Vanax TBSI
Vanax ns
Vulkacit NZ
Vulkacit NZ/EG

Inchi: InChI=1S/C11H14N2S2/c1-11(2,3)13-15-10-12-8-6-4-5-7-9(8)14-10/h4-7,13H,1-3H3

InchiKey: IUJLOAKJZQBENM-UHFFFAOYSA-N

Formula: C11H14N2S2

SMILES: CC(C)(C)NSc1nc2ccccc2s1

Mol. weight [g/mol]: 238.37

CAS: 95-31-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.09		Crippen Method
logp	3.692		Crippen Method
mcvol	179.590	ml/mol	McGowan Method
tf	382.45	K	Solubility of N-tert-Butylbenzothiazole-2-sulfenamide in Several Pure and Binary Solvents

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Solubility of N-tert-Butylbenzothiazole-2-sulfenamide in Several Pure and Binary Solvents:	https://www.doi.org/10.1021/acs.jced.8b00954
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C95318&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tf:	Normal melting (fusion) point