2(3H)-Benzothiazolethione

Other names:

1,3-Benzothiazole-2-thione
2-Benzothiazolinethione
2-Benzothiazolyl mercaptan
2-MBT
2-Mercaptobenzothiazole (2-MBT)
2-Mercaptobenzthiazole
2-Mercptobenzothiazole
2-Merkaptobenzotiazol
2-Merkaptobenzthiazol
2-benzothiazolethiol
2-mercaptobenzothiazole
ACCEL M
AG 63
Accelerator M
Accelerator Mercapto
BENZOTHIAZOLETHIOL
Benzo[d]thiazole-2-thiol
Benzothiazole, 2-mercapto-
Benzothiazole, mercapto-
Benzothiazole-2-thione
Captax
Dermacid
Ekagom G
Kaptaks
Kaptax
MBT
Mebetizole
Mebithizol
Mercaptobenzothiazol
Mercaptobenzothiazole
Mercaptobenzthiazole
Mertax
NCI-C56519
Nocceler M
Nuodeb 84
Pennac mbt powder
Perkacit MBT
Pneumax MBT
Rokon
Rotax

	Royal MBT
	Soxinol M
	Sulfadene
	Thiotax
	USAF GY-3
	USAF XR-29
	Vulkacit M
	Vulkacit Mercapto
	Vulkacit Mercapto/C
	benzothiazole-2-thiol
Inchi:	InChI=1S/C7H5NS2/c9-7-8-5-3-1-2-4-6(5)10-7/h1-4H,(H,8,9)
InchiKey:	YXIWHUQXZSMYRE-UHFFFAOYSA-N
Formula:	C7H5NS2
SMILES:	Sc1nc2ccccc2s1
Mol. weight [g/mol]:	167.26

Physical Properties

Property code	Value	Unit	Source
hfus	20.56	kJ/mol	Combustion energies and formation enthalpies of 2-SH-benzazoles
ie	7.99	eV	NIST Webbook
log10ws	-3.18		Aqueous Solubility Prediction Method
log10ws	-3.18		Estimated Solubility Method
logp	2.585		Crippen Method
mcvol	113.250	ml/mol	McGowan Method
rinpol	1944.00		NIST Webbook
rinpol	1944.00		NIST Webbook
tb	528.72	K	Cheméo Relay (1.0)
tf	454.75 ± 0.30	K	NIST Webbook
tf	455.15 ± 0.20	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hfust	20.56	kJ/mol	453.50	NIST Webbook

hfust	22.30 ± 0.20	kJ/mol	455.90	NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Cheméo Relay (1.0):	
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Cheméo Relay (1.0, beta):	
Thermodynamic functions for solubility of 2-mercaptobenzothiazole in eleven pure organic solvents at temperatures from 273.15 K to 318.15 K and mixing properties of solutions:	https://www.doi.org/10.1016/j.jct.2017.05.013
KDB:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1890
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Combustion energies and formation enthalpies of 2-SH-benzazoles:	https://www.doi.org/10.1016/j.jct.2008.02.018
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C149304&Units=SI
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt

Legend

hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point