

2-Mercaptobenzothiazole

Other names:

- 1,3-Benzothiazole-2-thione
- 2(3H)-BENZOTHIAZOLETHIONE
- 2-Benzothiazolethiol
- 2-Benzothiazolinethione
- 2-Benzothiazolyl mercaptan
- 2-MBT
- 2-Mercaptobenzothiazole (2-MBT)
- 2-Mercaptobenzthiazole
- 2-Mercptobenzothiazole
- 2-Merkaptobenzotiazol
- 2-Merkaptobenzthiazol
- 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]: 167.25
CAS: 149-30-4

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
rinpole	1944.00		NIST Webbook
rinpole	1944.00		NIST Webbook
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

Sources

Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C149304&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Combustion energies and formation enthalpies of 2-SH-benzazoles:	https://www.doi.org/10.1016/j.jct.2008.02.018
Thermodynamic functions for solubility of 2-mercaptobenzothiazole in eleven	https://www.doi.org/10.1016/j.jct.2017.05.013
organic solvents at temperatures	https://www.cheric.org/files/research/kdb/mol/mol1890.mol
from 273.15 K to 318.15 K and mixing	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
properties of solutions.	

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
tf:	Normal melting (fusion) point

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