4,5-DIMETHYL-2-THIAZOLETHIOL

Other names: 2(3H)-Thiazolethione, 4,5-dimethyl-
4-[5-Dimethyl-2-thiazolethiol
4,5-dimethylthiazole-2(3H)-thione
Inchi: InChI=1S/C5H7NS2/c1-3-4(2)8-5(7)6-3/h1-2H3,(H,6,7)
InchiKey: KKHBRTFQIYIHEI-UHFFFAOYSA-N
Formula: C5H7NS2
SMILES: Cc1nc(S)sc1C
Mol. weight [g/mol]: 145.25

Physical Properties

Property code	Value	Unit	Source
ie	7.56 ± 0.03	eV	NIST Webbook
logp	2.049		Crippen Method
mcvol	104.530	ml/mol	McGowan Method
tf	379.79	K	Cheméo Relay (1.0)

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C5351519&Units=SI
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):

Legend

ie: Ionization energy
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
tf: Normal melting (fusion) point