2-ISOBUTYL-4-METHYLTHIAZOLE

Other names: 2-iso-Butyl-4-methylthiazole
Thiazole, 2-isobutyl-4-methyl
Inchi: InChI=1S/C8H13NS/c1-6(2)4-8-9-7(3)5-10-8/h5-6H,4H2,1-3H3
InchiKey: JBUCYVMFLWLDIO-UHFFFAOYSA-N
Formula: C8H13NS
SMILES: Cc1csc(CC(C)C)n1
Mol. weight [g/mol]: 155.27

Physical Properties

Property code	Value	Unit	Source
logp	2.650		Crippen Method
mcvol	130.450	ml/mol	McGowan Method
rinpol	1086.00		NIST Webbook
rinpol	1086.00		NIST Webbook
ripol	1420.00		NIST Webbook
ripol	1420.00		NIST Webbook
tb	451.95	K	Cheméo Relay (1.0)
tf	220.41	K	Cheméo Relay (1.0)

Sources

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):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C61323248&Units=SI

Legend

logp: Octanol/Water partition coefficient

mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point