

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

Latest version available from:

<https://www.cheméo.com/cid/40-250-9/2-ISOBUTYL-4-METHYLTHIAZOLE.pdf>

Generated by Cheméo on 2026-07-22 02:29:12.84096996 +0000 UTC m=+198448.682855340.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.