

Thiazole, 4-methyl-2-(1-methylethyl)-

Other names: Thiazole, 2-isopropyl-4-methyl-
2-Isopropyl-4-methylthiazole
2-Isopropyl-4-methyl-1,3-thiazole
Thiazole, 4-methyl-2-isopropyl

Inchi: InChI=1S/C7H11NS/c1-5(2)7-8-6(3)4-9-7/h4-5H,1-3H3

InchiKey: OFLXNHNYPQPQKW-UHFFFAOYSA-N

Formula: C7H11NS

SMILES: Cc1csc(C(C)C)n1

Mol. weight [g/mol]: 141.23

CAS: 15679-13-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.66		Crippen Method
logp	2.575		Crippen Method
mcvol	116.360	ml/mol	McGowan Method
rinpol	1021.00		NIST Webbook
rinpol	1022.00		NIST Webbook
rinpol	1000.00		NIST Webbook
rinpol	1000.00		NIST Webbook
ripol	1339.00		NIST Webbook
ripol	1339.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C15679137&Units=SI>

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
ripol:	Polar retention indices

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