

2-Isobutylthiazole

Other names:	Thiazole, 2-isobutyl- Thiazole, 2-(2-methylpropyl)-
Inchi:	InChI=1S/C7H11NS/c1-6(2)5-7-8-3-4-9-7/h3-4,6H,5H2,1-2H3
InchiKey:	CMPVUVUNJQERIT-UHFFFAOYSA-N
Formula:	C7H11NS
SMILES:	CC(C)Cc1nccs1
Mol. weight [g/mol]:	141.23
CAS:	18640-74-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.39		Crippen Method
logp	2.342		Crippen Method
mcvol	116.360	ml/mol	McGowan Method
rinpol	1010.00		NIST Webbook
rinpol	1010.00		NIST Webbook
rinpol	1043.00		NIST Webbook
rinpol	1020.00		NIST Webbook
rinpol	1010.00		NIST Webbook
rinpol	1013.00		NIST Webbook
rinpol	1010.00		NIST Webbook
ripol	1406.00		NIST Webbook
ripol	1404.00		NIST Webbook
ripol	1378.00		NIST Webbook
ripol	1396.00		NIST Webbook
ripol	1378.00		NIST Webbook
tb	453.20	K	NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C18640749&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
tb:	Normal Boiling Point Temperature

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