

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

Other names:	Thiazole, 4-isopropyl-2-methyl- 4-Isopropyl-2-methylthiazole 4-Isopropyl-2-methyl-1,3-thiazole 2-Methyl-4-(1-methylethyl)thiazole
Inchi:	InChI=1S/C7H11NS/c1-5(2)7-4-9-6(3)8-7/h4-5H,1-3H3
InchiKey:	SRTOJEUVLKLAGK-UHFFFAOYSA-N
Formula:	C7H11NS
SMILES:	<chem>Cc1nc(C(C)C)cs1</chem>
Mol. weight [g/mol]:	141.23
CAS:	32272-52-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.66		Crippen Method
logp	2.575		Crippen Method
mcvol	116.360	ml/mol	McGowan Method
ripol	1514.00		NIST Webbook

Sources

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=C32272529&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

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

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