

Thiazole, 5-ethyl-2,4-dimethyl-

Other names:	2,4-Dimethyl-5-ethylthiazole 5-Ethyl-2,4-dimethylthiazole
Inchi:	InChI=1S/C7H11NS/c1-4-7-5(2)8-6(3)9-7/h4H2,1-3H3
InchiKey:	DALUCNUGMDNXET-UHFFFAOYSA-N
Formula:	C7H11NS
SMILES:	CCc1sc(C)nc1C
Mol. weight [g/mol]:	141.23
CAS:	38205-61-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.75		Crippen Method
logp	2.322		Crippen Method
mcvol	116.360	ml/mol	McGowan Method
ripol	1072.00		NIST Webbook
ripol	1078.00		NIST Webbook
ripol	1048.00		NIST Webbook
ripol	1049.00		NIST Webbook
ripol	1072.00		NIST Webbook
ripol	1077.00		NIST Webbook
ripol	1072.00		NIST Webbook
ripol	1047.00		NIST Webbook
ripol	1078.00		NIST Webbook
ripol	1078.00		NIST Webbook
ripol	1428.00		NIST Webbook
ripol	1438.00		NIST Webbook
ripol	1435.00		NIST Webbook
ripol	1455.00		NIST Webbook
ripol	1450.00		NIST Webbook
ripol	1443.00		NIST Webbook
ripol	1428.00		NIST Webbook
ripol	1438.00		NIST Webbook
ripol	1439.00		NIST Webbook
ripol	1438.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C38205617&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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