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

Other names: 2-Ethyl-4,5-dimethylthiazole
4,5-Dimethyl-2-ethylthiazole
Inchi: InChI=1S/C7H11NS/c1-4-7-8-5(2)6(3)9-7/h4H2,1-3H3
InchiKey: BVOKJOZBJOWZNJ-UHFFFAOYSA-N
Formula: C7H11NS
SMILES: CCc1nc(C)c(C)s1
Mol. weight [g/mol]: 141.23
CAS: 873-64-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.75		Crippen Method
logp	2.322		Crippen Method
mcvol	116.360	ml/mol	McGowan Method
rinpol	1105.00		NIST Webbook
rinpol	1077.00		NIST Webbook
rinpol	1073.00		NIST Webbook
rinpol	1105.00		NIST Webbook
rinpol	1073.00		NIST Webbook
rinpol	1060.00		NIST Webbook
rinpol	1077.00		NIST Webbook
rinpol	1065.00		NIST Webbook
rinpol	1082.00		NIST Webbook
ripol	1439.00		NIST Webbook
ripol	1439.00		NIST Webbook
ripol	1441.00		NIST Webbook
ripol	1442.00		NIST Webbook
ripol	1429.00		NIST Webbook
ripol	1429.00		NIST Webbook
ripol	1439.00		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=C873643&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