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

Other names:	2,5-Dimethyl-4-ethylthiazole
	4-Ethyl-2,5-dimethylthiazole
Inchi:	InChI=1S/C7H11NS/c1-4-7-5(2)9-6(3)8-7/h4H2,1-3H3
InchiKey:	ZJGXJKFDKNNBTK-UHFFFAOYSA-N
Formula:	C7H11NS
SMILES:	CCc1nc(C)sc1C
Mol. weight [g/mol]:	141.23
CAS:	32272-57-4

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	1066.00		NIST Webbook
rinpol	1065.00		NIST Webbook
rinpol	1043.00		NIST Webbook
rinpol	1076.00		NIST Webbook
rinpol	1037.00		NIST Webbook
rinpol	1038.00		NIST Webbook
rinpol	1050.00		NIST Webbook
rinpol	1072.00		NIST Webbook
rinpol	1077.00		NIST Webbook
rinpol	1086.00		NIST Webbook
rinpol	1074.00		NIST Webbook
rinpol	1050.00		NIST Webbook
ripol	1398.00		NIST Webbook
ripol	1398.00		NIST Webbook
ripol	1419.00		NIST Webbook
ripol	1417.00		NIST Webbook
ripol	1426.00		NIST Webbook
ripol	1398.00		NIST Webbook
ripol	1438.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C32272574&Units=SI
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

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