4-Ethyl-5-methylthiazole

Other names: Thiazole, 4-ethyl-5-methyl-
Inchi: InChI=1S/C6H9NS/c1-3-6-5(2)8-4-7-6/h4H,3H2,1-2H3
InchiKey: QCIOXFPPEGZRFY-UHFFFAOYSA-N
Formula: C6H9NS
SMILES: CCc1ncsc1C
Mol. weight [g/mol]: 127.21
CAS: 52414-91-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.27		Crippen Method
logp	2.014		Crippen Method
mcvol	102.270	ml/mol	McGowan Method
rinpol	1010.00		NIST Webbook
rinpol	1005.00		NIST Webbook
rinpol	991.00		NIST Webbook
ripol	1401.00		NIST Webbook
ripol	1403.00		NIST Webbook
ripol	1412.00		NIST Webbook
ripol	1422.00		NIST Webbook
ripol	1424.00		NIST Webbook
ripol	1400.00		NIST Webbook
ripol	1401.00		NIST Webbook
ripol	1412.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C52414912&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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