2-Ethyl-4-methylthiazole

Other names: Thiazole, 2-ethyl-4-methyl-
2-Ethyl-4-methyl-1,3-thiazole
4-Methyl-2-ethylthiazole
Inchi: InChI=1S/C6H9NS/c1-3-6-7-5(2)4-8-6/h4H,3H2,1-2H3
InchiKey: VGRVKVGGUPOCMT-UHFFFAOYSA-N
Formula: C6H9NS
SMILES: CCc1nc(C)cs1
Mol. weight [g/mol]: 127.21
CAS: 15679-12-6

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	955.00		NIST Webbook
rinpol	970.00		NIST Webbook
rinpol	970.00		NIST Webbook
rinpol	964.00		NIST Webbook
rinpol	948.00		NIST Webbook
rinpol	948.00		NIST Webbook
rinpol	948.00		NIST Webbook
rinpol	948.00		NIST Webbook
ripol	1349.00		NIST Webbook
ripol	1349.00		NIST Webbook
ripol	1368.00		NIST Webbook
ripol	1322.00		NIST Webbook
ripol	1352.00		NIST Webbook
ripol	1331.00		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=C15679126&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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