2-Ethyl-5-methylthiazole

Other names:	5-Methyl-2-ethylthiazole
	Thiazole, 2-ethyl-5-methyl-
Inchi:	InChI=1S/C6H9NS/c1-3-6-7-4-5(2)8-6/h4H,3H2,1-2H3
InchiKey:	YXWWUNNKMJZIOW-UHFFFAOYSA-N
Formula:	C6H9NS
SMILES:	CCc1ncc(C)s1
Mol. weight [g/mol]:	127.21
CAS:	19961-53-6

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	1004.00		NIST Webbook
rinpol	974.00		NIST Webbook
rinpol	1004.00		NIST Webbook
rinpol	1001.00		NIST Webbook
rinpol	1004.00		NIST Webbook
rinpol	997.00		NIST Webbook
rinpol	997.00		NIST Webbook
ripol	1388.00		NIST Webbook
ripol	1388.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C19961536&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