

Thiazole, 2-ethyl-

Other names:	2-Ethylthiazole
Inchi:	InChI=1S/C5H7NS/c1-2-5-6-3-4-7-5/h3-4H,2H2,1H3
InchiKey:	CGZDWVZMOMDGBN-UHFFFAOYSA-N
Formula:	C5H7NS
SMILES:	CCc1nccs1
Mol. weight [g/mol]:	113.18
CAS:	15679-09-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.80		Crippen Method
logp	1.706		Crippen Method
mcvol	88.180	ml/mol	McGowan Method
ripol	869.00		NIST Webbook
ripol	867.00		NIST Webbook
ripol	869.00		NIST Webbook
ripol	879.00		NIST Webbook
ripol	867.00		NIST Webbook
ripol	906.00		NIST Webbook
ripol	887.00		NIST Webbook
ripol	867.00		NIST Webbook
ripol	1319.00		NIST Webbook
ripol	1317.00		NIST Webbook
ripol	1319.00		NIST Webbook
ripol	1300.00		NIST Webbook
ripol	1319.00		NIST Webbook
ripol	1265.00		NIST Webbook
ripol	1304.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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