

5-Ethylthiazole

Other names:	Thiazole, 5-ethyl-
Inchi:	InChI=1S/C5H7NS/c1-2-5-3-6-4-7-5/h3-4H,2H2,1H3
InchiKey:	ASAMCDOTLOUAAR-UHFFFAOYSA-N
Formula:	C5H7NS
SMILES:	CCc1cnsc1
Mol. weight [g/mol]:	113.18
CAS:	17626-73-2

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	917.00		NIST Webbook
ripol	955.00		NIST Webbook
ripol	959.00		NIST Webbook
ripol	940.00		NIST Webbook
ripol	914.00		NIST Webbook
ripol	914.00		NIST Webbook
ripol	951.00		NIST Webbook
ripol	959.00		NIST Webbook
ripol	914.00		NIST Webbook
ripol	951.00		NIST Webbook
ripol	917.00		NIST Webbook
ripol	1315.00		NIST Webbook
ripol	1315.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C17626732&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemed.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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