4-Ethyl-1,3-thiazole

Other names:	4-Ethylthiazole
	Thiazole, 4-ethyl-
Inchi:	InChI=1S/C5H7NS/c1-2-5-3-7-4-6-5/h3-4H,2H2,1H3
InchiKey:	CGOVTZGCKPMLMN-UHFFFAOYSA-N
Formula:	C5H7NS
SMILES:	CCc1cscn1
Mol. weight [g/mol]:	113.18
CAS:	17626-72-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.80		Crippen Method
logp	1.706		Crippen Method
mcvol	88.180	ml/mol	McGowan Method
rinpol	873.00		NIST Webbook
rinpol	873.00		NIST Webbook
rinpol	880.00		NIST Webbook
rinpol	880.00		NIST Webbook
rinpol	916.00		NIST Webbook
rinpol	873.00		NIST Webbook
ripol	1281.00		NIST Webbook
ripol	1281.00		NIST Webbook
ripol	1281.00		NIST Webbook

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C17626721&Units=SI

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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