

Isothiazole, 4,5-dimethyl-

Other names:	4,5-Dimethylisothiazole
Inchi:	InChI=1S/C5H7NS/c1-4-3-6-7-5(4)2/h3H,1-2H3
InchiKey:	SPRVGONRQZESPA-UHFFFAOYSA-N
Formula:	C5H7NS
SMILES:	Cc1cnsc1C
Mol. weight [g/mol]:	113.18
CAS:	27330-47-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.95		Crippen Method
logp	1.760		Crippen Method
mcvol	88.180	ml/mol	McGowan Method
ripol	974.00		NIST Webbook
ripol	988.00		NIST Webbook
ripol	974.00		NIST Webbook
ripol	988.00		NIST Webbook
ripol	974.00		NIST Webbook
ripol	1400.00		NIST Webbook
ripol	1400.00		NIST Webbook
ripol	1423.00		NIST Webbook
ripol	1423.00		NIST Webbook
ripol	1400.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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=C27330478&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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