

Isothiazole, trimethyl-

Other names:	3,4,5-Trimethylisothiazole Trimethylisothiazole
Inchi:	InChI=1S/C6H9NS/c1-4-5(2)7-8-6(4)3/h1-3H3
InchiKey:	GGRRWFKQGMXXQS-UHFFFAOYSA-N
Formula:	C6H9NS
SMILES:	Cc1nsc(C)c1C
Mol. weight [g/mol]:	127.21
CAS:	39228-36-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.42		Crippen Method
logp	2.068		Crippen Method
mcvol	102.270	ml/mol	McGowan Method
ripol	1394.00		NIST Webbook
ripol	1394.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C39228369&Units=SI
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
ripol:	Polar retention indices

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