

Isothiazole, 5-methyl-

Other names:	5-Methylisothiazole
Inchi:	InChI=1S/C4H5NS/c1-4-2-3-5-6-4/h2-3H,1H3
InchiKey:	LBBKWEDRPDGXPM-UHFFFAOYSA-N
Formula:	C4H5NS
SMILES:	Cc1ccns1
Mol. weight [g/mol]:	99.15
CAS:	693-97-0

Physical Properties

Property code	Value	Unit	Source
ie	9.65	eV	NIST Webbook
log10ws	-1.47		Crippen Method
logp	1.452		Crippen Method
mcvol	74.090	ml/mol	McGowan Method
rinpol	820.00		NIST Webbook
rinpol	820.00		NIST Webbook
rinpol	862.00		NIST Webbook
rinpol	862.00		NIST Webbook
ripol	1282.00		NIST Webbook
ripol	1299.00		NIST Webbook
ripol	1282.00		NIST Webbook
tb	418.20	K	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C693970&Units=SI
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

Legend

ie:	Ionization energy
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
tb:	Normal Boiling Point Temperature

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