

5-Thiazoleethanol, 4-methyl-

Other names:	Hemineurine
	MHT
	4-Methyl-5-(«beta»-Hydroxyethyl)thiazole
	4-Methyl-5-(2-hydroxyethyl)thiazole
	4-Methyl-5-hydroxyethylthiazole
	4-Methyl-5-thiazoleethanol
	4-Methyl-5-thiazolethanol
	5-(Hydroxyethyl)-4-methylthiazole
	5-(2-Hydroxyethyl)-4-methylthiazole
	Sulfurol
	Thiazole, 5-(2-hydroxyethyl)-4-methyl
	2-(4-Methylthiazole-5-yl)ethanol
	4-Methyl-5-thiazolyethanol
	NSC 23262
	5-(2-hydroxyethyl)-4-methylthiazole (sulfurol)
	2-(4-methylthiazol-5-yl)ethanol
Inchi:	InChI=1S/C6H9NOS/c1-5-6(2-3-8)9-4-7-5/h4,8H,2-3H2,1H3
InchiKey:	BKAWJIRCKVUVED-UHFFFAOYSA-N
Formula:	C6H9NOS
SMILES:	Cc1ncsc1CCO
Mol. weight [g/mol]:	143.21
CAS:	137-00-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.54		Crippen Method
logp	0.986		Crippen Method
mcvol	108.140	ml/mol	McGowan Method
rinpol	1241.00		NIST Webbook
rinpol	1247.00		NIST Webbook
rinpol	1283.00		NIST Webbook
rinpol	1246.00		NIST Webbook
rinpol	1241.00		NIST Webbook
rinpol	1271.00		NIST Webbook
ripol	2275.00		NIST Webbook
ripol	2275.00		NIST Webbook
ripol	2275.00		NIST Webbook

ripol	2309.00	NIST Webbook
ripol	2311.00	NIST Webbook
ripol	2302.00	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	408.20	K	0.90	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C137008&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
tbrp:	Boiling point at reduced pressure

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