

2-Thiazolamine, 4-methyl-

Other names:	Thiazole, 2-amino-4-methyl- Normotiroide 2-Amino-4-methylthiazole 4-Methyl-2-aminothiazole 4-Methyl-2-thiazolamine 4-Methyl-2-thiazolylamine Nomortiroide 4-Methyl-1,3-thiazol-2-amine 2-Amino-4-methyl-1,3-thiazole 4-methylthiazol-2-ylamine
Inchi:	InChI=1S/C4H6N2S/c1-3-2-7-4(5)6-3/h2H,1H3,(H2,5,6)
InchiKey:	OUQMXTJYCAJLGO-UHFFFAOYSA-N
Formula:	C4H6N2S
SMILES:	Cc1csc(N)n1
Mol. weight [g/mol]:	114.17
CAS:	1603-91-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.10		Crippen Method
logp	1.034		Crippen Method
mcvol	84.070	ml/mol	McGowan Method
ripol	1414.00		NIST Webbook
ripol	1414.00		NIST Webbook
tb	504.70	K	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	398.20	K	2.70	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=C1603914&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure

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