

Thiazole, 5-ethenyl-4-methyl-

Other names:	5-Ethenyl-4-methylthiazole 4-Methyl-5-vinylthiazole Thiazole, 4-methyl-5-vinyl- 5-Vinyl-4-methylthiazole
Inchi:	InChI=1S/C6H7NS/c1-3-6-5(2)7-4-8-6/h3-4H,1H2,2H3
InchiKey:	QUAMMXIRDIIGDJ-UHFFFAOYSA-N
Formula:	C6H7NS
SMILES:	C=Cc1scnc1C
Mol. weight [g/mol]:	125.19
CAS:	1759-28-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.29		Crippen Method
logp	2.095		Crippen Method
mcvol	97.970	ml/mol	McGowan Method
ripol	1029.00		NIST Webbook
ripol	1011.00		NIST Webbook
ripol	1056.00		NIST Webbook
ripol	999.00		NIST Webbook
ripol	1056.00		NIST Webbook
ripol	1512.00		NIST Webbook
ripol	1524.00		NIST Webbook
ripol	1560.00		NIST Webbook
ripol	1512.00		NIST Webbook
ripol	1500.00		NIST Webbook
ripol	1500.00		NIST Webbook
ripol	1518.00		NIST Webbook
ripol	1518.00		NIST Webbook
ripol	1560.00		NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
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Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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=C1759280&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
tbrp:	Boiling point at reduced pressure

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