

Thiazole, 5-methyl-

Other names:	5-Methylthiazole
Inchi:	InChI=1S/C4H5NS/c1-4-2-5-3-6-4/h2-3H,1H3
InchiKey:	RLYUNPNLXMSXAX-UHFFFAOYSA-N
Formula:	C4H5NS
SMILES:	Cc1cnsc1
Mol. weight [g/mol]:	99.15
CAS:	3581-89-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.47		Crippen Method
logp	1.452		Crippen Method
mcvol	74.090	ml/mol	McGowan Method
ripol	854.00		NIST Webbook
ripol	865.00		NIST Webbook
ripol	840.00		NIST Webbook
ripol	820.00		NIST Webbook
ripol	825.00		NIST Webbook
ripol	814.00		NIST Webbook
ripol	814.00		NIST Webbook
ripol	865.00		NIST Webbook
ripol	869.00		NIST Webbook
ripol	846.00		NIST Webbook
ripol	865.00		NIST Webbook
ripol	854.00		NIST Webbook
ripol	1331.00		NIST Webbook
ripol	1318.00		NIST Webbook
ripol	1318.00		NIST Webbook
ripol	1324.00		NIST Webbook
ripol	1318.00		NIST Webbook
tf	232.74 ± 0.05	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hfust	7.65	kJ/mol	232.80	NIST Webbook
hfust	7.65	kJ/mol	232.80	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	414.70	K	99.30	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3581893&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

hfust:	Enthalpy of fusion at a given temperature
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
tf:	Normal melting (fusion) point

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