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:	Cc1cncs1
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
rinpol	814.00		NIST Webbook
rinpol	854.00		NIST Webbook
rinpol	814.00		NIST Webbook
rinpol	869.00		NIST Webbook
rinpol	846.00		NIST Webbook
rinpol	865.00		NIST Webbook
rinpol	865.00		NIST Webbook
rinpol	865.00		NIST Webbook
rinpol	840.00		NIST Webbook
rinpol	820.00		NIST Webbook
rinpol	825.00		NIST Webbook
rinpol	854.00		NIST Webbook
ripol	1318.00		NIST Webbook
ripol	1324.00		NIST Webbook
ripol	1318.00		NIST Webbook
ripol	1318.00		NIST Webbook
ripol	1331.00		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

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=C3581893&Units=SI

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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