2-Methylthiazole

Inchi: InChI=1S/C4H5NS/c1-4-5-2-3-6-4/h2-3H,1H3
InchiKey: VZWOXDYRBDIHMA-UHFFFAOYSA-N
Formula: C4H5NS
SMILES: Cc1nccs1
Mol. weight [g/mol]: 99.15
CAS: 3581-87-1

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	1218.00		NIST Webbook
ripol	1218.00		NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.42228e+01
Coeff. B	-3.23985e+03
Coeff. C	-6.38240e+01
Temperature range (K), min.	296.32
Temperature range (K), max.	427.39

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=U121691&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pvap:	Vapor pressure
ripol:	Polar retention indices

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