Thiazole, 2-methyl-

Other names: 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
affp	930.60	kJ/mol	NIST Webbook
basg	898.70	kJ/mol	NIST Webbook
log10ws	-1.47		Crippen Method
logp	1.452		Crippen Method
mcvol	74.090	ml/mol	McGowan Method
rinpol	777.00		NIST Webbook
rinpol	790.00		NIST Webbook
rinpol	791.00		NIST Webbook
rinpol	777.00		NIST Webbook
rinpol	810.00		NIST Webbook
rinpol	763.00		NIST Webbook
rinpol	780.00		NIST Webbook
rinpol	808.00		NIST Webbook
rinpol	777.00		NIST Webbook
rinpol	815.00		NIST Webbook
rinpol	815.00		NIST Webbook
rinpol	778.00		NIST Webbook
rinpol	832.00		NIST Webbook
rinpol	783.00		NIST Webbook
rinpol	819.00		NIST Webbook
ripol	1239.00		NIST Webbook
ripol	1222.00		NIST Webbook
ripol	1220.00		NIST Webbook
ripol	1239.00		NIST Webbook
ripol	1228.00		NIST Webbook
ripol	1260.00		NIST Webbook
ripol	1260.00		NIST Webbook

ripol	1250.00		NIST Webbook
ripol	1243.00		NIST Webbook
ripol	1241.00		NIST Webbook
ripol	1268.00		NIST Webbook
ripol	1250.00		NIST Webbook
ripol	1265.00		NIST Webbook
ripol	1256.00		NIST Webbook
sl	211.90	J/mol×K	NIST Webbook
sl	211.88	J/mol×K	NIST Webbook
sl	211.88	J/mol×K	NIST Webbook
tb	401.95 ± 0.25	K	NIST Webbook
tb	401.70	K	NIST Webbook
tf	248.43 ± 0.05	K	NIST Webbook
tt	248.43 ± 0.02	K	NIST Webbook
tt	246.53 ± 0.02	K	NIST Webbook
tt	248.43 ± 0.02	K	NIST Webbook
tt	246.50 ± 0.20	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpl	150.70	J/mol×K	298.15	NIST Webbook
cpl	150.67	J/mol×K	298.15	NIST Webbook
cpl	150.67	J/mol×K	298.15	NIST Webbook
hfust	12.16	kJ/mol	248.60	NIST Webbook
hvapt	39.40	kJ/mol	377.50	NIST Webbook
hvapt	40.00	kJ/mol	373.00	NIST Webbook

Sources

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=C3581871&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

affp:	Proton affinity
basg:	Gas basicity
cpl:	Liquid phase heat capacity
hfust:	Enthalpy of fusion at a given temperature
hvapt:	Enthalpy of vaporization 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
sl:	Liquid phase molar entropy at standard conditions
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature