4-Methylthiazole

Other names: Thiazole, 4-methyl-
Inchi: InChI=1S/C4H5NS/c1-4-2-6-3-5-4/h2-3H,1H3
InchiKey: QMHIMXFNBOYPND-UHFFFAOYSA-N
Formula: C4H5NS
SMILES: Cc1cscn1
Mol. weight [g/mol]: 99.15
CAS: 693-95-8

Physical Properties

Property code	Value	Unit	Source
chl	-2958.80 ± 0.59	kJ/mol	NIST Webbook
hf	111.80 ± 0.88	kJ/mol	NIST Webbook
hfl	67.91 ± 0.75	kJ/mol	NIST Webbook
hvap	43.80 ± 0.20	kJ/mol	NIST Webbook
hvap	43.80 ± 0.20	kJ/mol	NIST Webbook
log10ws	-1.47		Crippen Method
logp	1.452		Crippen Method
mcvol	74.090	ml/mol	McGowan Method
rinpol	811.00		NIST Webbook
rinpol	823.00		NIST Webbook
rinpol	823.00		NIST Webbook
rinpol	821.00		NIST Webbook
rinpol	836.00		NIST Webbook
rinpol	836.00		NIST Webbook
rinpol	821.00		NIST Webbook
rinpol	777.00		NIST Webbook
rinpol	793.00		NIST Webbook
rinpol	789.00		NIST Webbook
rinpol	861.00		NIST Webbook
rinpol	861.00		NIST Webbook
rinpol	836.00		NIST Webbook
rinpol	830.00		NIST Webbook
rinpol	786.00		NIST Webbook
rinpol	802.00		NIST Webbook
rinpol	786.00		NIST Webbook
rinpol	830.00		NIST Webbook
rinpol	798.00		NIST Webbook

rinpol	791.00		NIST Webbook
rinpol	786.00		NIST Webbook
rinpol	786.00		NIST Webbook
rinpol	800.00		NIST Webbook
rinpol	828.00		NIST Webbook
rinpol	795.00		NIST Webbook
rinpol	831.00		NIST Webbook
rinpol	831.00		NIST Webbook
ripol	1278.00		NIST Webbook
ripol	1270.00		NIST Webbook
ripol	1287.00		NIST Webbook
ripol	1265.00		NIST Webbook
ripol	1263.00		NIST Webbook
ripol	1284.00		NIST Webbook
ripol	1286.00		NIST Webbook
ripol	1272.00		NIST Webbook
ripol	1270.00		NIST Webbook
ripol	1274.00		NIST Webbook
ripol	1270.00		NIST Webbook
ripol	1279.00		NIST Webbook
ripol	1278.00		NIST Webbook
ripol	1304.00		NIST Webbook
ripol	1304.00		NIST Webbook
ripol	1287.00		NIST Webbook
ripol	1297.00		NIST Webbook
ripol	1312.00		NIST Webbook
ripol	1297.00		NIST Webbook
ripol	1265.00		NIST Webbook
ripol	1265.00		NIST Webbook
ripol	1284.00		NIST Webbook
ripol	1280.00		NIST Webbook
ripol	1278.00		NIST Webbook
ripol	1288.00		NIST Webbook
tb	406.36 ± 0.25	K	NIST Webbook
tb	406.70	K	NIST Webbook
tf	229.02 ± 0.05	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hfust	8.90	kJ/mol	229.10	NIST Webbook

hfust	8.90	kJ/mol	229.10	NIST Webbook
hvapt	40.80	kJ/mol	377.00	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=C693958&Units=SI

Legend

chl:	Standard liquid enthalpy of combustion
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase enthalpy of formation at standard conditions
hfust:	Enthalpy of fusion at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
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
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point