Thiazole, 2,4-dimethyl-

Other names: 2,4-Dimethylthiazole
Inchi: InChI=1S/C5H7NS/c1-4-3-7-5(2)6-4/h3H,1-2H3
InchiKey: OBSLLHNATPQFMJ-UHFFFAOYSA-N
Formula: C5H7NS
SMILES: Cc1csc(C)n1
Mol. weight [g/mol]: 113.18
CAS: 541-58-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.95		Crippen Method
logp	1.760		Crippen Method
mcvol	88.180	ml/mol	McGowan Method
rinpol	887.00		NIST Webbook
rinpol	857.00		NIST Webbook
rinpol	858.00		NIST Webbook
rinpol	860.00		NIST Webbook
rinpol	883.00		NIST Webbook
rinpol	887.00		NIST Webbook
rinpol	892.00		NIST Webbook
rinpol	860.00		NIST Webbook
rinpol	868.00		NIST Webbook
rinpol	899.00		NIST Webbook
rinpol	857.00		NIST Webbook
rinpol	858.00		NIST Webbook
rinpol	883.00		NIST Webbook
rinpol	861.00		NIST Webbook
rinpol	869.00		NIST Webbook
rinpol	887.00		NIST Webbook
ripol	1256.00		NIST Webbook
ripol	1285.00		NIST Webbook
ripol	1293.00		NIST Webbook
ripol	1283.00		NIST Webbook
ripol	1268.00		NIST Webbook
ripol	1285.00		NIST Webbook
ripol	1258.00		NIST Webbook
ripol	1271.00		NIST Webbook

ripol	1291.00		NIST Webbook
ripol	1291.00		NIST Webbook
ripol	1282.00		NIST Webbook
tf	222.84 ± 0.05	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hfust	2.90	kJ/mol	222.90	NIST Webbook
hfust	2.90	kJ/mol	222.90	NIST Webbook
hvapt	42.00	kJ/mol	389.00	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	344.70	K	6.70	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=C541582&Units=SI

Legend

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
tbrp:	Boiling point at reduced pressure
tf:	Normal melting (fusion) point