

Thiazole, 2,4,5-trimethyl-

Other names:	2,4,5-Trimethylthiazole Trimethylthiazole
Inchi:	InChI=1S/C6H9NS/c1-4-5(2)8-6(3)7-4/h1-3H3
InchiKey:	BAMPVSWRQZNDQC-UHFFFAOYSA-N
Formula:	C6H9NS
SMILES:	Cc1nc(C)c(C)s1
Mol. weight [g/mol]:	127.21
CAS:	13623-11-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.42		Crippen Method
logp	2.068		Crippen Method
mcvol	102.270	ml/mol	McGowan Method
rinpol	973.00		NIST Webbook
rinpol	973.00		NIST Webbook
rinpol	997.00		NIST Webbook
rinpol	997.00		NIST Webbook
rinpol	1028.00		NIST Webbook
rinpol	981.00		NIST Webbook
rinpol	974.00		NIST Webbook
rinpol	973.00		NIST Webbook
rinpol	969.00		NIST Webbook
rinpol	969.00		NIST Webbook
rinpol	981.00		NIST Webbook
rinpol	965.00		NIST Webbook
rinpol	997.00		NIST Webbook
rinpol	972.00		NIST Webbook
rinpol	995.00		NIST Webbook
rinpol	1000.00		NIST Webbook
rinpol	976.00		NIST Webbook
rinpol	996.00		NIST Webbook
rinpol	997.00		NIST Webbook
rinpol	1007.00		NIST Webbook
rinpol	990.00		NIST Webbook
rinpol	997.00		NIST Webbook
rinpol	990.00		NIST Webbook

ripol	974.00			NIST Webbook
ripol	1007.00			NIST Webbook
ripol	972.00			NIST Webbook
ripol	969.00			NIST Webbook
ripol	997.00			NIST Webbook
ripol	990.00			NIST Webbook
ripol	997.00			NIST Webbook
ripol	995.00			NIST Webbook
ripol	1000.00			NIST Webbook
ripol	1380.00			NIST Webbook
ripol	1387.00			NIST Webbook
ripol	1394.00			NIST Webbook
ripol	1362.00			NIST Webbook
ripol	1358.00			NIST Webbook
ripol	1367.00			NIST Webbook
ripol	1380.00			NIST Webbook
ripol	1370.00			NIST Webbook
ripol	1367.00			NIST Webbook
ripol	1398.00			NIST Webbook
ripol	1394.00			NIST Webbook
ripol	1398.00			NIST Webbook
ripol	1377.00			NIST Webbook
ripol	1390.00			NIST Webbook
ripol	1362.00			NIST Webbook
ripol	1358.00			NIST Webbook
ripol	1390.00			NIST Webbook
ripol	1380.00			NIST Webbook
ripol	1387.00			NIST Webbook
ripol	1385.00			NIST Webbook
ripol	1377.00			NIST Webbook
ripol	1366.00			NIST Webbook
ripol	1378.00			NIST Webbook
ripol	1362.00			NIST Webbook
ripol	1380.00			NIST Webbook
ripol	1380.00			NIST Webbook
tf	240.69 ± 0.05		K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hfust	9.00	kJ/mol	240.70	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	439.70	K	95.70	NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C13623115&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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