

# Thiazole, 4,5-dimethyl-

<b>Other names:</b>	4,5-Dimethylthiazole
<b>Inchi:</b>	InChI=1S/C5H7NS/c1-4-5(2)7-3-6-4/h3H,1-2H3
<b>InchiKey:</b>	UWSONZCNXUSTKW-UHFFFAOYSA-N
<b>Formula:</b>	C5H7NS
<b>SMILES:</b>	Cc1ncsc1C
<b>Mol. weight [g/mol]:</b>	113.18
<b>CAS:</b>	3581-91-7

## 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	906.00		NIST Webbook
rinpol	941.00		NIST Webbook
rinpol	928.00		NIST Webbook
rinpol	922.00		NIST Webbook
rinpol	907.00		NIST Webbook
rinpol	910.00		NIST Webbook
rinpol	928.00		NIST Webbook
rinpol	951.00		NIST Webbook
rinpol	947.00		NIST Webbook
rinpol	906.00		NIST Webbook
rinpol	933.00		NIST Webbook
rinpol	926.00		NIST Webbook
rinpol	941.00		NIST Webbook
rinpol	910.00		NIST Webbook
rinpol	937.00		NIST Webbook
rinpol	945.00		NIST Webbook
rinpol	945.00		NIST Webbook
rinpol	933.00		NIST Webbook
rinpol	929.00		NIST Webbook
rinpol	909.00		NIST Webbook
rinpol	907.00		NIST Webbook
rinpol	910.00		NIST Webbook
rinpol	917.00		NIST Webbook
rinpol	910.00		NIST Webbook

ripol	941.00	NIST Webbook
ripol	907.00	NIST Webbook
ripol	929.00	NIST Webbook
ripol	936.00	NIST Webbook
ripol	1376.00	NIST Webbook
ripol	1374.00	NIST Webbook
ripol	1374.00	NIST Webbook
ripol	1372.00	NIST Webbook
ripol	1409.00	NIST Webbook
ripol	1409.00	NIST Webbook
ripol	1377.00	NIST Webbook
ripol	1378.00	NIST Webbook
ripol	1360.00	NIST Webbook
ripol	1341.00	NIST Webbook
ripol	1371.00	NIST Webbook
ripol	1359.00	NIST Webbook
ripol	1372.00	NIST Webbook
ripol	1379.00	NIST Webbook
ripol	1381.00	NIST Webbook
ripol	1324.00	NIST Webbook
ripol	1379.00	NIST Webbook
ripol	1378.00	NIST Webbook
ripol	1359.00	NIST Webbook
ripol	1379.00	NIST Webbook
ripol	1324.00	NIST Webbook
ripol	1370.00	NIST Webbook

## Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	431.20	K	98.90	NIST Webbook

## Sources

- NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=C3581917&Units=SI>
- Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
- Crippen Method:** [https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)
- McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>

# Legend

<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume
<b>rinpol:</b>	Non-polar retention indices
<b>ripol:</b>	Polar retention indices
<b>tbrp:</b>	Boiling point at reduced pressure

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