

Oxazole, trimethyl-

Other names:	Trimethyloxazole 2,4,5-Trimethyloxazole Oxazole, 2,4,5-trimethyl
Inchi:	InChI=1S/C6H9NO/c1-4-5(2)8-6(3)7-4/h1-3H3
InchiKey:	ZRLDBDZSLLGDOX-UHFFFAOYSA-N
Formula:	C6H9NO
SMILES:	Cc1nc(C)c(C)o1
Mol. weight [g/mol]:	111.14
CAS:	20662-84-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.40		Crippen Method
logp	1.600		Crippen Method
mcvol	91.790	ml/mol	McGowan Method
rinpol	828.00		NIST Webbook
rinpol	843.00		NIST Webbook
rinpol	843.00		NIST Webbook
rinpol	848.00		NIST Webbook
rinpol	843.00		NIST Webbook
rinpol	850.00		NIST Webbook
rinpol	853.00		NIST Webbook
rinpol	829.00		NIST Webbook
rinpol	846.00		NIST Webbook
rinpol	857.00		NIST Webbook
rinpol	843.00		NIST Webbook
rinpol	826.00		NIST Webbook
rinpol	851.00		NIST Webbook
rinpol	863.00		NIST Webbook
rinpol	847.00		NIST Webbook
rinpol	856.60		NIST Webbook
rinpol	822.00		NIST Webbook
rinpol	823.00		NIST Webbook
rinpol	827.00		NIST Webbook
rinpol	824.00		NIST Webbook
rinpol	855.00		NIST Webbook
rinpol	829.00		NIST Webbook

ripol	830.00		NIST Webbook
ripol	852.00		NIST Webbook
ripol	1206.00		NIST Webbook
ripol	1200.00		NIST Webbook
ripol	1200.00		NIST Webbook
ripol	1188.00		NIST Webbook
ripol	1193.00		NIST Webbook
ripol	1193.00		NIST Webbook
ripol	1197.00		NIST Webbook
ripol	1193.00		NIST Webbook
ripol	1224.00		NIST Webbook
ripol	1190.00		NIST Webbook
ripol	1188.00		NIST Webbook
ripol	1215.00		NIST Webbook
ripol	1209.00		NIST Webbook
ripol	1209.00		NIST Webbook
ripol	1200.00		NIST Webbook
ripol	1204.00		NIST Webbook
ripol	1214.00		NIST Webbook
ripol	1214.00		NIST Webbook
ripol	1197.00		NIST Webbook
ripol	1211.00		NIST Webbook
ripol	1190.00		NIST Webbook
ripol	1179.00		NIST Webbook
ripol	1191.00		NIST Webbook
ripol	1200.00		NIST Webbook
ripol	1192.00		NIST Webbook
ripol	1192.00		NIST Webbook
ripol	1194.00		NIST Webbook
ripol	1194.00		NIST Webbook
ripol	1200.00		NIST Webbook
ripol	1191.00		NIST Webbook
tb	406.70	K	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=C20662844&Units=SI>

Legend

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

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<https://www.chemeo.com/cid/20-899-2/Oxazole-trimethyl.pdf>

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