

Isoxazole, trimethyl-

Other names:	Trimethylisoxazole 3,4,5-Trimethylisoxazole Isoxazole, 3,4,5-trimethyl- USAF CS-1340
Inchi:	InChI=1S/C6H9NO/c1-4-5(2)7-8-6(4)3/h1-3H3
InchiKey:	MGHKWBQZEBMFOH-UHFFFAOYSA-N
Formula:	C6H9NO
SMILES:	Cc1noc(C)c1C
Mol. weight [g/mol]:	111.14
CAS:	10557-82-1

Physical Properties

Property code	Value	Unit	Source
hf	-20.00 ± 4.20	kJ/mol	NIST Webbook
hfl	-70.20 ± 3.30	kJ/mol	NIST Webbook
hvap	50.00 ± 2.00	kJ/mol	NIST Webbook
log10ws	-6.40		Crippen Method
logp	1.600		Crippen Method
mvol	91.790	ml/mol	McGowan Method

Sources

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=C10557821&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase enthalpy of formation at standard conditions

hvap: Enthalpy of vaporization at standard conditions
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume

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