Isoxazole, 3,5-dimethyl-

Other names:	U 21221
	3,5-Dimethylisoxazole
	3,5-Dimethylisooxazole
	DMI
	3,5-Dwumetyloizoksazolu
Inchi:	InChI=1S/C5H7NO/c1-4-3-5(2)7-6-4/h3H,1-2H3
InchiKey:	FICAQKBMCKEFDI-UHFFFAOYSA-N
Formula:	C5H7NO
SMILES:	Cc1cc(C)on1
Mol. weight [g/mol]:	97.12
CAS:	300-87-8

Physical Properties

Property code	Value	Unit	Source
chl	-2905.00 ± 2.90	kJ/mol	NIST Webbook
hf	-18.00 ± 4.00	kJ/mol	NIST Webbook
hfl	-63.10 ± 3.10	kJ/mol	NIST Webbook
hvap	45.00 ± 2.00	kJ/mol	NIST Webbook
log10ws	-5.92		Crippen Method
logp	1.291		Crippen Method
mcvol	77.700	ml/mol	McGowan Method
rinpol	801.00		NIST Webbook
rinpol	801.00		NIST Webbook
ripol	1135.00		NIST Webbook
ripol	1135.00		NIST Webbook
tb	416.20	K	NIST Webbook

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=C300878&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

chl:	Standard liquid enthalpy of combustion
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
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature