

Isoxazole, 4-(chloromethyl)-3,5-dimethyl-

Other names:	4-(Chloromethyl)-3,5-dimethylisoxazole
Inchi:	InChI=1S/C6H8CINO/c1-4-6(3-7)5(2)9-8-4/h3H2,1-2H3
InchiKey:	NIFAUKBQIAURIM-UHFFFAOYSA-N
Formula:	C6H8CINO
SMILES:	Cc1noc(C)c1CCl
Mol. weight [g/mol]:	145.59
CAS:	19788-37-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.95		Crippen Method
logp	2.030		Crippen Method
mcvol	104.030	ml/mol	McGowan Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	360.70	K	1.00	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=C19788375&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcpvol:	McGowan's characteristic volume
tbrp:	Boiling point at reduced pressure

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