

4-CHLOROMETHYL-3,5-DIMETHYLISOXAZOLE

Other names:	4-(Chloromethyl)-3,5-dimethylisoxazole
Inchi:	InChI=1S/C6H8ClNO/c1-4-6(3-7)5(2)9-8-4/h3H2,1-2H3
InchiKey:	NIFAUKBQIAURIM-UHFFFAOYSA-N
Formula:	C6H8ClNO
SMILES:	Cc1noc(C)c1CCl
Mol. weight [g/mol]:	145.59

Physical Properties

Property code	Value	Unit	Source
hf	-79.47	kJ/mol	Cheméo Relay (1.0)
hvap	56.73	kJ/mol	Cheméo Relay (1.0)
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
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C19788375&Units=SI
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

hf:	Enthalpy of formation at standard conditions
h_{vap}:	Enthalpy of vaporization at standard conditions
log_p:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
t_{brp}:	Boiling point at reduced pressure

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