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
hvap:	Enthalpy of vaporization at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tbrp:	Boiling point at reduced pressure