

Chloroacetyl isocyanate

Other names:	Chloroacetyl isocyanate 2-Chloroacetyl isocyanate Acetyl isocyanate, chloro-
Inchi:	InChI=1S/C3H2CINO2/c4-1-3(7)5-2-6/h1H2
InchiKey:	MOVMEFHWBOWMFU-UHFFFAOYSA-N
Formula:	C3H2CINO2
SMILES:	O=C=NC(=O)CCI
Mol. weight [g/mol]:	119.51
CAS:	4461-30-7

Physical Properties

Property code	Value	Unit	Source
hf	-238.98	kJ/mol	Joback Method
hvap	42.94	kJ/mol	Joback Method
log10ws	-4.50		Crippen Method
logp	0.088		Crippen Method
mvol	74.190	ml/mol	McGowan Method
pc	5058.59	kPa	Joback Method
tb	426.01	K	Joback Method
tc	628.43	K	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4461307&Units=SI

Legend

hf:	Enthalpy of formation at standard conditions
h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀ws:	Log ₁₀ of Water solubility in mol/l
log_p:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature

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