

CHLOROMETHYL 9-CHLORONONANOATE

Other names:	9-Chlorononanoic acid, chloromethyl ester
Inchi:	InChI=1S/C10H18Cl2O2/c11-8-6-4-2-1-3-5-7-10(13)14-9-12/h1-9H2
InchiKey:	AAVUFTKCHHFPHZ-UHFFFAOYSA-N
Formula:	C10H18Cl2O2
SMILES:	O=C(CCCCCCCCCI)OCCI
Mol. weight [g/mol]:	241.16

Physical Properties

Property code	Value	Unit	Source
hf	-617.77	kJ/mol	Cheméo Relay (1.0)
hfus	32.84	kJ/mol	Joback Method
hvap	76.00	kJ/mol	Cheméo Relay (1.0)
ie	10.05	eV	Cheméo Relay (1.0)
log10ws	-4.31		Cheméo Relay (1.0)
logp	3.695		Crippen Method
mcvol	183.680	ml/mol	McGowan Method
pc	2054.89	kPa	Joback Method
tb	545.20	K	Cheméo Relay (1.0)
tc	743.18	K	Cheméo Relay (1.0)
tf	279.13	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	427.35	J/mol×K	579.35	Joback Method
cpg	440.37	J/mol×K	609.70	Joback Method
cpg	452.81	J/mol×K	640.06	Joback Method
cpg	464.67	J/mol×K	670.41	Joback Method
cpg	475.97	J/mol×K	700.77	Joback Method
cpg	486.72	J/mol×K	731.12	Joback Method
cpg	496.91	J/mol×K	761.47	Joback Method
dvisc	0.0024726	Pa×s	334.46	Joback Method
dvisc	0.0013060	Pa×s	375.27	Joback Method
dvisc	0.0007818	Pa×s	416.09	Joback Method

dvisc	0.0005129	Pa×s	456.90	Joback Method
dvisc	0.0003606	Pa×s	497.72	Joback Method
dvisc	0.0002675	Pa×s	538.53	Joback Method
dvisc	0.0002069	Pa×s	579.35	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C80418786&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point

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