CHLOROMETHYL 3-CHLORONONANOATE

Other names: 3-Chlorononanoic acid, chloromethyl ester
Inchi: InChI=1S/C10H18Cl2O2/c1-2-3-4-5-6-9(12)7-10(13)14-8-11/h9H,2-8H2,1H3
InchiKey: QADYLIOQVFEZKX-UHFFFAOYSA-N
Formula: C10H18Cl2O2
SMILES: CCCCCCC(Cl)CC(=O)OCCl
Mol. weight [g/mol]: 241.16

Physical Properties

Property code	Value	Unit	Source
hf	-619.10	kJ/mol	Cheméo Relay (1.0)
hfus	29.31	kJ/mol	Joback Method
hvap	68.41	kJ/mol	Cheméo Relay (1.0)
logp	3.694		Crippen Method
mcvol	183.680	ml/mol	McGowan Method
rinpol	1521.00		NIST Webbook
rinpol	1526.00		NIST Webbook
rinpol	1526.00		NIST Webbook
rinpol	1529.00		NIST Webbook
ripol	2059.00		NIST Webbook
ripol	2059.00		NIST Webbook
ripol	2084.00		NIST Webbook
ripol	2081.00		NIST Webbook
tb	529.09	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	427.73	J/mol×K	578.91	Joback Method
cpg	441.05	J/mol×K	609.83	Joback Method
cpg	453.75	J/mol×K	640.75	Joback Method
cpg	465.85	J/mol×K	671.67	Joback Method
cpg	477.36	J/mol×K	702.58	Joback Method
cpg	488.28	J/mol×K	733.50	Joback Method
cpg	498.63	J/mol×K	764.42	Joback Method

dvisc	0.0032066	Pa×s	319.46	Joback Method
dvisc	0.0015197	Pa×s	362.70	Joback Method
dvisc	0.0008444	Pa×s	405.94	Joback Method
dvisc	0.0005254	Pa×s	449.19	Joback Method
dvisc	0.0003553	Pa×s	492.43	Joback Method
dvisc	0.0002560	Pa×s	535.67	Joback Method
dvisc	0.0001937	Pa×s	578.91	Joback Method

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=C80418720&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature