Chloromethyl 4-chlorodecanoate

Other names: 4-Chlorodecanoic acid, chloromethyl ester
Inchi: InChI=1S/C11H20Cl2O2/c1-2-3-4-5-6-10(13)7-8-11(14)15-9-12/h10H,2-9H2,1H3
InchiKey: LDNMSCDSUKAAMZ-UHFFFAOYSA-N
Formula: C11H20Cl2O2
SMILES: CCCCCCC(Cl)CCC(=O)OCCl
Mol. weight [g/mol]: 255.18
CAS: 80418-81-1

Physical Properties

Property code	Value	Unit	Source
gf	-218.48	kJ/mol	Joback Method
hf	-551.93	kJ/mol	Joback Method
hfus	31.90	kJ/mol	Joback Method
hvap	57.62	kJ/mol	Joback Method
log10ws	-4.20		Crippen Method
logp	4.084		Crippen Method
mcvol	197.770	ml/mol	McGowan Method
pc	1900.26	kPa	Joback Method
rinpol	1654.00		NIST Webbook
rinpol	1658.00		NIST Webbook
rinpol	1650.00		NIST Webbook
rinpol	1650.00		NIST Webbook
rinpol	1664.00		NIST Webbook
ripol	2227.00		NIST Webbook
ripol	2193.00		NIST Webbook
ripol	2212.00		NIST Webbook
ripol	2193.00		NIST Webbook
ripol	2233.00		NIST Webbook
tb	601.79	K	Joback Method
tc	785.44	K	Joback Method
tf	330.73	K	Joback Method
vc	0.767	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	476.80	J/mol×K	601.79	Joback Method
cpg	490.81	J/mol×K	632.40	Joback Method
cpg	504.16	J/mol×K	663.01	Joback Method
cpg	516.86	J/mol×K	693.62	Joback Method
cpg	528.94	J/mol×K	724.22	Joback Method
cpg	540.40	J/mol×K	754.83	Joback Method
cpg	551.25	J/mol×K	785.44	Joback Method
dvisc	0.0029863	Pa×s	330.73	Joback Method
dvisc	0.0013948	Pa×s	375.91	Joback Method
dvisc	0.0007671	Pa×s	421.08	Joback Method
dvisc	0.0004737	Pa×s	466.26	Joback Method
dvisc	0.0003185	Pa×s	511.44	Joback Method
dvisc	0.0002284	Pa×s	556.61	Joback Method
dvisc	0.0001722	Pa×s	601.79	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C80418811&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

Legend

cpg: Ideal gas heat capacity

dvisc: Dynamic viscosity

gf: Standard Gibbs free energy of formation

hf: Enthalpy of formation at standard conditions

hfus: Enthalpy of fusion at standard conditions

hvap: Enthalpy of vaporization at standard conditions

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume