6-Chlorodecanoic acid, chloromethyl ester

Inchi: InChI=1S/C11H20Cl2O2/c1-2-3-6-10(13)7-4-5-8-11(14)15-9-12/h10H,2-9H2,1H3
InchiKey: MMRVINVMGHJPGW-UHFFFAOYSA-N
Formula: C11H20Cl2O2
SMILES: CCCCC(Cl)CCCCC(=O)OCCl
Mol. weight [g/mol]: 255.18

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	1690.00		NIST Webbook
rinpol	1678.00		NIST Webbook
rinpol	1684.00		NIST Webbook
rinpol	1672.00		NIST Webbook
rinpol	1672.00		NIST Webbook
ripol	2234.00		NIST Webbook
ripol	2257.00		NIST Webbook
ripol	2276.00		NIST Webbook
ripol	2277.00		NIST Webbook
ripol	2234.00		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

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=R249528&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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