

Chloromethyl 9-chlorodecanoate

Other names:	9-Chlorodecanoic acid, chloromethyl ester
Inchi:	InChI=1S/C11H20Cl2O2/c1-10(13)7-5-3-2-4-6-8-11(14)15-9-12/h10H,2-9H2,1H3
InchiKey:	KPSTVHFMJIDEGU-UHFFFAOYSA-N
Formula:	C11H20Cl2O2
SMILES:	CC(Cl)CCCCCCCC(=O)OCCI
Mol. weight [g/mol]:	255.18
CAS:	80418-86-6

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	1696.00		NIST Webbook
rinpol	1709.00		NIST Webbook
rinpol	1704.00		NIST Webbook
rinpol	1719.00		NIST Webbook
rinpol	1696.00		NIST Webbook
ripol	2274.00		NIST Webbook
ripol	2320.00		NIST Webbook
ripol	2321.00		NIST Webbook
ripol	2299.00		NIST Webbook
ripol	2274.00		NIST Webbook
tb	601.79	K	Joback Method
tc	785.44	K	Joback Method
tf	330.73	K	Joback Method
vc	0.767	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	476.80	J/molxK	601.79	Joback Method
cpg	540.40	J/molxK	754.83	Joback Method
cpg	528.94	J/molxK	724.22	Joback Method
cpg	516.86	J/molxK	693.62	Joback Method
cpg	504.16	J/molxK	663.01	Joback Method
cpg	490.81	J/molxK	632.40	Joback Method
cpg	551.25	J/molxK	785.44	Joback Method
dvisc	0.0001722	Paxs	601.79	Joback Method
dvisc	0.0002284	Paxs	556.61	Joback Method
dvisc	0.0003185	Paxs	511.44	Joback Method
dvisc	0.0004737	Paxs	466.26	Joback Method
dvisc	0.0007671	Paxs	421.08	Joback Method
dvisc	0.0013948	Paxs	375.91	Joback Method
dvisc	0.0029863	Paxs	330.73	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=C80418866&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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

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