2-Chlorodecanoic acid, methyl ester

Inchi: InChI=1S/C11H21ClO2/c1-3-4-5-6-7-8-9-10(12)11(13)14-2/h10H,3-9H2,1-2H3
InchiKey: SOBKMRUKIGDINL-UHFFFAOYSA-N
Formula: C11H21ClO2
SMILES: CCCCCCCCC(Cl)C(=O)OC
Mol. weight [g/mol]: 220.74

Physical Properties

Property code	Value	Unit	Source
gf	-206.55	kJ/mol	Joback Method
hf	-536.19	kJ/mol	Joback Method
hfus	27.71	kJ/mol	Joback Method
hvap	53.23	kJ/mol	Joback Method
log10ws	-3.55		Crippen Method
logp	3.517		Crippen Method
mcvol	185.530	ml/mol	McGowan Method
pc	1963.07	kPa	Joback Method
rinpol	1451.00		NIST Webbook
rinpol	1459.00		NIST Webbook
ripol	1869.00		NIST Webbook
ripol	1820.00		NIST Webbook
tb	564.36	K	Joback Method
tc	743.50	K	Joback Method
tf	300.81	K	Joback Method
vc	0.719	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	446.93	J/mol×K	564.36	Joback Method
cpg	461.63	J/mol×K	594.22	Joback Method
cpg	475.70	J/mol×K	624.07	Joback Method
cpg	489.15	J/mol×K	653.93	Joback Method
cpg	501.98	J/mol×K	683.78	Joback Method
cpg	514.22	J/mol×K	713.64	Joback Method

cpg	525.87	J/mol×K	743.50	Joback Method
dvisc	0.0036823	Pa×s	300.81	Joback Method
dvisc	0.0016303	Pa×s	344.74	Joback Method
dvisc	0.0008677	Pa×s	388.66	Joback Method
dvisc	0.0005249	Pa×s	432.59	Joback Method
dvisc	0.0003484	Pa×s	476.51	Joback Method
dvisc	0.0002478	Pa×s	520.44	Joback Method
dvisc	0.0001859	Pa×s	564.36	Joback Method

Sources

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=R309145&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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