Chloromethyl undecanoate

Other names: Undecanoic acid, chloromethyl ester
Inchi: InChI=1S/C12H23ClO2/c1-2-3-4-5-6-7-8-9-10-12(14)15-11-13/h2-11H2,1H3
InchiKey: BDZBWJLRACXOET-UHFFFAOYSA-N
Formula: C12H23ClO2
SMILES: CCCCCCCCCCC(=O)OCCl
Mol. weight [g/mol]: 234.76
CAS: 77877-96-4

Physical Properties

Property code	Value	Unit	Source
gf	-195.69	kJ/mol	Joback Method
hf	-551.55	kJ/mol	Joback Method
hfus	33.82	kJ/mol	Joback Method
hvap	55.85	kJ/mol	Joback Method
log10ws	-4.36		Crippen Method
logp	4.257		Crippen Method
mcvol	199.620	ml/mol	McGowan Method
pc	1793.94	kPa	Joback Method
rinpol	1581.00		NIST Webbook
ripol	1990.00		NIST Webbook
tb	587.68	K	Joback Method
tc	762.26	K	Joback Method
tf	327.08	K	Joback Method
vc	0.780	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	496.42	J/mol×K	587.68	Joback Method
cpg	565.36	J/mol×K	733.17	Joback Method
cpg	552.80	J/mol×K	704.07	Joback Method
cpg	539.64	J/mol×K	674.97	Joback Method
cpg	525.87	J/mol×K	645.87	Joback Method
cpg	511.47	J/mol×K	616.78	Joback Method

cpg	577.32	J/mol×K	762.26	Joback Method
dvisc	0.0001781	Pa×s	587.68	Joback Method
dvisc	0.0002330	Pa×s	544.25	Joback Method
dvisc	0.0003194	Pa×s	500.81	Joback Method
dvisc	0.0004650	Pa×s	457.38	Joback Method
dvisc	0.0007323	Pa×s	413.95	Joback Method
dvisc	0.0012830	Pa×s	370.51	Joback Method
dvisc	0.0026085	Pa×s	327.08	Joback Method

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C77877964&Units=SI

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