Chloromethyl 6-chloroundecanoate

Other names: 6-Chloroundecanoic acid, chloromethyl ester
Inchi: InChI=1S/C12H22Cl2O2/c1-2-3-4-7-11(14)8-5-6-9-12(15)16-10-13/h11H,2-10H2,1H3
InchiKey: NHURGYSRXYAHKJ-UHFFFAOYSA-N
Formula: C12H22Cl2O2
SMILES: CCCCCC(Cl)CCCCC(=O)OCCl
Mol. weight [g/mol]: 269.21
CAS: 80418-92-4

Physical Properties

Property code	Value	Unit	Source
gf	-210.06	kJ/mol	Joback Method
hf	-572.57	kJ/mol	Joback Method
hfus	34.49	kJ/mol	Joback Method
hvap	59.84	kJ/mol	Joback Method
log10ws	-4.62		Crippen Method
logp	4.474		Crippen Method
mcvol	211.860	ml/mol	McGowan Method
pc	1750.67	kPa	Joback Method
rinpol	1775.00		NIST Webbook
rinpol	1783.00		NIST Webbook
rinpol	1770.00		NIST Webbook
rinpol	1796.00		NIST Webbook
ripol	2350.00		NIST Webbook
ripol	2350.00		NIST Webbook
ripol	2373.00		NIST Webbook
ripol	2369.00		NIST Webbook
tb	624.67	K	Joback Method
tc	806.72	K	Joback Method
tf	342.00	K	Joback Method
vc	0.824	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	527.44	J/mol×K	624.67	Joback Method
cpg	593.73	J/mol×K	776.38	Joback Method
cpg	581.80	J/mol×K	746.04	Joback Method
cpg	569.22	J/mol×K	715.70	Joback Method
cpg	555.97	J/mol×K	685.35	Joback Method
cpg	542.05	J/mol×K	655.01	Joback Method
cpg	605.03	J/mol×K	806.72	Joback Method
dvisc	0.0001524	Pa×s	624.67	Joback Method
dvisc	0.0002028	Pa×s	577.56	Joback Method
dvisc	0.0002840	Pa×s	530.45	Joback Method
dvisc	0.0004246	Pa×s	483.33	Joback Method
dvisc	0.0006925	Pa×s	436.22	Joback Method
dvisc	0.0012714	Pa×s	389.11	Joback Method
dvisc	0.0027597	Pa×s	342.00	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C80418924&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

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