Chloromethyl 11-chloroundecanoate

Other names: 11-Chloroundecanoic acid, chloromethyl ester
Inchi: InChI=1S/C12H22Cl2O2/c13-10-8-6-4-2-1-3-5-7-9-12(15)16-11-14/h1-11H2
InchiKey: ZLIBDGLPYRUFEI-UHFFFAOYSA-N
Formula: C12H22Cl2O2
SMILES: O=C(CCCCCCCCCCCl)OCCl
Mol. weight [g/mol]: 269.21
CAS: 80418-97-9

Physical Properties

Property code	Value	Unit	Source
gf	-207.62	kJ/mol	Joback Method
hf	-567.29	kJ/mol	Joback Method
hfus	38.02	kJ/mol	Joback Method
hvap	60.23	kJ/mol	Joback Method
log10ws	-4.51		Crippen Method
logp	4.476		Crippen Method
mcvol	211.860	ml/mol	McGowan Method
pc	1739.01	kPa	Joback Method
rinpol	1885.00		NIST Webbook
rinpol	1847.00		NIST Webbook
rinpol	1861.00		NIST Webbook
rinpol	1856.00		NIST Webbook
ripol	2502.00		NIST Webbook
ripol	2499.00		NIST Webbook
ripol	2471.00		NIST Webbook
tb	625.11	K	Joback Method
tc	804.22	K	Joback Method
tf	357.00	K	Joback Method
vc	0.830	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	527.01	J/mol×K	625.11	Joback Method

cpg	541.35	J/mol×K	654.96	Joback Method
cpg	555.02	J/mol×K	684.81	Joback Method
cpg	568.05	J/mol×K	714.67	Joback Method
cpg	580.44	J/mol×K	744.52	Joback Method
cpg	592.21	J/mol×K	774.37	Joback Method
cpg	603.37	J/mol×K	804.22	Joback Method
dvisc	0.0021690	Pa×s	357.00	Joback Method
dvisc	0.0011095	Pa×s	401.69	Joback Method
dvisc	0.0006490	Pa×s	446.37	Joback Method
dvisc	0.0004186	Pa×s	491.05	Joback Method
dvisc	0.0002905	Pa×s	535.74	Joback Method
dvisc	0.0002132	Pa×s	580.42	Joback Method
dvisc	0.0001636	Pa×s	625.11	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=C80418979&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