2-chloroethyl undecanoate

Inchi: InChI=1S/C13H25ClO2/c1-2-3-4-5-6-7-8-9-10-13(15)16-12-11-14/h2-12H2,1H3
InchiKey: XFCXIVMYZNRAFR-UHFFFAOYSA-N
Formula: C13H25ClO2
SMILES: CCCCCCCCCCC(=O)OCCCl
Mol. weight [g/mol]: 248.79

Physical Properties

Property code	Value	Unit	Source
gf	-187.27	kJ/mol	Joback Method
hf	-572.19	kJ/mol	Joback Method
hfus	36.41	kJ/mol	Joback Method
hvap	58.07	kJ/mol	Joback Method
log10ws	-4.28		Crippen Method
logp	4.299		Crippen Method
mcvol	213.710	ml/mol	McGowan Method
pc	1656.49	kPa	Joback Method
rinpol	1693.00		NIST Webbook
rinpol	1701.00		NIST Webbook
rinpol	1701.00		NIST Webbook
rinpol	1693.00		NIST Webbook
rinpol	1697.00		NIST Webbook
rinpol	1712.00		NIST Webbook
rinpol	1699.00		NIST Webbook
rinpol	1693.00		NIST Webbook
ripol	2200.00		NIST Webbook
ripol	2181.00		NIST Webbook
ripol	2200.00		NIST Webbook
ripol	2158.00		NIST Webbook
ripol	2168.00		NIST Webbook
ripol	2168.00		NIST Webbook
ripol	2182.00		NIST Webbook
ripol	2169.00		NIST Webbook
ripol	2169.00		NIST Webbook
ripol	2158.00		NIST Webbook
tb	610.56	K	Joback Method
tc	784.07	K	Joback Method
tf	338.35	K	Joback Method

vc	0.837	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	547.83	J/mol×K	610.56	Joback Method
cpg	619.38	J/mol×K	755.15	Joback Method
cpg	606.37	J/mol×K	726.24	Joback Method
cpg	592.72	J/mol×K	697.32	Joback Method
cpg	578.43	J/mol×K	668.40	Joback Method
cpg	563.46	J/mol×K	639.48	Joback Method
cpg	631.77	J/mol×K	784.07	Joback Method
dvisc	0.0001590	Pa×s	610.56	Joback Method
dvisc	0.0002089	Pa×s	565.19	Joback Method
dvisc	0.0002878	Pa×s	519.82	Joback Method
dvisc	0.0004215	Pa×s	474.45	Joback Method
dvisc	0.0006691	Pa×s	429.09	Joback Method
dvisc	0.0011849	Pa×s	383.72	Joback Method
dvisc	0.0024461	Pa×s	338.35	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=R30894&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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