1-Undecanol, 2-chloro, acetate

Other names: 2-Chloroundecyl acetate
Inchi: InChI=1S/C13H25ClO2/c1-3-4-5-6-7-8-9-10-13(14)11-16-12(2)15/h13H,3-11H2,1-2H3
InchiKey: DTMBCKHHJOBNSN-UHFFFAOYSA-N
Formula: C13H25ClO2
SMILES: CCCCCCCCCC(Cl)COC(C)=O
Mol. weight [g/mol]: 248.79

Physical Properties

Property code	Value	Unit	Source
gf	-189.71	kJ/mol	Joback Method
hf	-577.47	kJ/mol	Joback Method
hfus	32.89	kJ/mol	Joback Method
hvap	57.69	kJ/mol	Joback Method
log10ws	-4.39		Crippen Method
logp	4.298		Crippen Method
mcvol	213.710	ml/mol	McGowan Method
pc	1667.33	kPa	Joback Method
rinpol	1637.00		NIST Webbook
rinpol	1646.00		NIST Webbook
rinpol	1649.00		NIST Webbook
rinpol	1643.00		NIST Webbook
rinpol	1646.00		NIST Webbook
ripol	2099.00		NIST Webbook
ripol	2080.00		NIST Webbook
ripol	2086.00		NIST Webbook
ripol	2072.00		NIST Webbook
ripol	2070.00		NIST Webbook
tb	610.12	K	Joback Method
tc	786.44	K	Joback Method
tf	323.35	K	Joback Method
vc	0.831	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	548.21	J/mol×K	610.12	Joback Method
cpg	564.14	J/mol×K	639.51	Joback Method
cpg	579.37	J/mol×K	668.89	Joback Method
cpg	593.91	J/mol×K	698.28	Joback Method
cpg	607.77	J/mol×K	727.67	Joback Method
cpg	620.96	J/mol×K	757.05	Joback Method
cpg	633.51	J/mol×K	786.44	Joback Method
dvisc	0.0031957	Pa×s	323.35	Joback Method
dvisc	0.0013781	Pa×s	371.14	Joback Method
dvisc	0.0007200	Pa×s	418.94	Joback Method
dvisc	0.0004297	Pa×s	466.74	Joback Method
dvisc	0.0002822	Pa×s	514.53	Joback Method
dvisc	0.0001991	Pa×s	562.33	Joback Method
dvisc	0.0001484	Pa×s	610.12	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=R33797&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