1-Dodecanol, 3-chloro, acetate

Other names: 3-Chlorododecyl acetate
Inchi: InChI=1S/C14H27ClO2/c1-3-4-5-6-7-8-9-10-14(15)11-12-17-13(2)16/h14H,3-12H2,1-2H3
InchiKey: XVNQJPWIRWZBTO-UHFFFAOYSA-N
Formula: C14H27ClO2
SMILES: CCCCCCCCCC(Cl)CCOC(C)=O
Mol. weight [g/mol]: 262.82

Physical Properties

Property code	Value	Unit	Source
gf	-181.29	kJ/mol	Joback Method
hf	-598.11	kJ/mol	Joback Method
hfus	35.48	kJ/mol	Joback Method
hvap	59.91	kJ/mol	Joback Method
log10ws	-4.81		Crippen Method
logp	4.688		Crippen Method
mcvol	227.800	ml/mol	McGowan Method
pc	1543.92	kPa	Joback Method
rinpol	1767.00		NIST Webbook
rinpol	1764.00		NIST Webbook
rinpol	1761.00		NIST Webbook
rinpol	1767.00		NIST Webbook
ripol	2213.00		NIST Webbook
ripol	2225.00		NIST Webbook
ripol	2230.00		NIST Webbook
ripol	2236.00		NIST Webbook
tb	633.00	K	Joback Method
tc	808.33	K	Joback Method
tf	334.62	K	Joback Method
vc	0.886	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	601.12	J/mol×K	633.00	Joback Method

cpg	617.58	J/mol×K	662.22	Joback Method
cpg	633.29	J/mol×K	691.44	Joback Method
cpg	648.28	J/mol×K	720.66	Joback Method
cpg	662.56	J/mol×K	749.89	Joback Method
cpg	676.15	J/mol×K	779.11	Joback Method
cpg	689.06	J/mol×K	808.33	Joback Method
dvisc	0.0029420	Pa×s	334.62	Joback Method
dvisc	0.0012536	Pa×s	384.35	Joback Method
dvisc	0.0006495	Pa×s	434.08	Joback Method
dvisc	0.0003852	Pa×s	483.81	Joback Method
dvisc	0.0002518	Pa×s	533.54	Joback Method
dvisc	0.0001770	Pa×s	583.27	Joback Method
dvisc	0.0001315	Pa×s	633.00	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=R33121&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