1-Dodecanol, 12-chloro, acetate

Other names: 12-Chlorododecyl acetate
Inchi: InChI=1S/C14H27ClO2/c1-14(16)17-13-11-9-7-5-3-2-4-6-8-10-12-15/h2-13H2,1H3
InchiKey: RQEURDOLMGSSEM-UHFFFAOYSA-N
Formula: C14H27ClO2
SMILES: CC(=O)OCCCCCCCCCCCCCl
Mol. weight [g/mol]: 262.82

Physical Properties

Property code	Value	Unit	Source
gf	-178.85	kJ/mol	Joback Method
hf	-592.83	kJ/mol	Joback Method
hfus	39.00	kJ/mol	Joback Method
hvap	60.30	kJ/mol	Joback Method
log10ws	-4.70		Crippen Method
logp	4.689		Crippen Method
mcvol	227.800	ml/mol	McGowan Method
pc	1534.26	kPa	Joback Method
rinpol	1859.00		NIST Webbook
rinpol	1865.00		NIST Webbook
rinpol	1868.00		NIST Webbook
rinpol	1869.00		NIST Webbook
rinpol	1859.00		NIST Webbook
ripol	2416.00		NIST Webbook
ripol	2390.00		NIST Webbook
ripol	2429.00		NIST Webbook
ripol	2407.00		NIST Webbook
ripol	2390.00		NIST Webbook
tb	633.44	K	Joback Method
tc	806.19	K	Joback Method
tf	349.62	K	Joback Method
vc	0.892	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	600.72	J/mol×K	633.44	Joback Method
cpg	616.89	J/mol×K	662.23	Joback Method
cpg	632.35	J/mol×K	691.02	Joback Method
cpg	647.12	J/mol×K	719.81	Joback Method
cpg	661.20	J/mol×K	748.60	Joback Method
cpg	674.62	J/mol×K	777.39	Joback Method
cpg	687.38	J/mol×K	806.19	Joback Method
dvisc	0.0022752	Pa×s	349.62	Joback Method
dvisc	0.0010865	Pa×s	396.92	Joback Method
dvisc	0.0006073	Pa×s	444.23	Joback Method
dvisc	0.0003797	Pa×s	491.53	Joback Method
dvisc	0.0002578	Pa×s	538.83	Joback Method
dvisc	0.0001863	Pa×s	586.14	Joback Method
dvisc	0.0001413	Pa×s	633.44	Joback Method

Sources

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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R33096&Units=SI

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