1-Decanol, 5-chloro, acetate

Other names: 5-Chlorodecyl acetate
Inchi: InChI=1S/C12H23ClO2/c1-3-4-5-8-12(13)9-6-7-10-15-11(2)14/h12H,3-10H2,1-2H3
InchiKey: ZEFARAPWFWHPRY-UHFFFAOYSA-N
Formula: C12H23ClO2
SMILES: CCCCCC(Cl)CCCCOC(C)=O
Mol. weight [g/mol]: 234.76

Physical Properties

Property code	Value	Unit	Source
gf	-198.13	kJ/mol	Joback Method
hf	-556.83	kJ/mol	Joback Method
hfus	30.30	kJ/mol	Joback Method
hvap	55.46	kJ/mol	Joback Method
log10ws	-3.97		Crippen Method
logp	3.907		Crippen Method
mcvol	199.620	ml/mol	McGowan Method
pc	1806.16	kPa	Joback Method
rinpol	1573.00		NIST Webbook
rinpol	1578.00		NIST Webbook
rinpol	1580.00		NIST Webbook
rinpol	1582.00		NIST Webbook
rinpol	1573.00		NIST Webbook
ripol	2051.00		NIST Webbook
ripol	2051.00		NIST Webbook
ripol	2055.00		NIST Webbook
ripol	2067.00		NIST Webbook
ripol	2072.00		NIST Webbook
tb	587.24	K	Joback Method
tc	764.85	K	Joback Method
tf	312.08	K	Joback Method
vc	0.774	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	496.78	J/mol×K	587.24	Joback Method
cpg	566.97	J/mol×K	735.25	Joback Method
cpg	554.22	J/mol×K	705.64	Joback Method
cpg	540.84	J/mol×K	676.04	Joback Method
cpg	526.82	J/mol×K	646.44	Joback Method
cpg	512.13	J/mol×K	616.84	Joback Method
cpg	579.10	J/mol×K	764.85	Joback Method
dvisc	0.0001665	Pa×s	587.24	Joback Method
dvisc	0.0002228	Pa×s	541.38	Joback Method
dvisc	0.0003146	Pa×s	495.52	Joback Method
dvisc	0.0004765	Pa×s	449.66	Joback Method
dvisc	0.0007932	Pa×s	403.80	Joback Method
dvisc	0.0015046	Pa×s	357.94	Joback Method
dvisc	0.0034450	Pa×s	312.08	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R33028&Units=SI
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

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

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