

1-Dodecanol, 7-chloro, acetate

Other names:	7-Chlorododecyl acetate
Inchi:	InChI=1S/C14H27ClO2/c1-3-4-7-10-14(15)11-8-5-6-9-12-17-13(2)16/h14H,3-12H2,1-2H3
InchiKey:	YNDUCIRZZOERET-UHFFFAOYSA-N
Formula:	C14H27ClO2
SMILES:	CCCCC(Cl)CCCCCOC(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	1789.00		NIST Webbook
rinpol	1786.00		NIST Webbook
rinpol	1791.00		NIST Webbook
rinpol	1791.00		NIST Webbook
rinpol	1786.00		NIST Webbook
ripol	2262.00		NIST Webbook
ripol	2287.00		NIST Webbook
ripol	2280.00		NIST Webbook
ripol	2275.00		NIST Webbook
ripol	2262.00		NIST Webbook
tb	633.00	K	Joback Method
tc	808.33	K	Joback Method
tf	334.62	K	Joback Method
vc	0.886	m ³ /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	Paxs	334.62	Joback Method
dvisc	0.0012536	Paxs	384.35	Joback Method
dvisc	0.0006495	Paxs	434.08	Joback Method
dvisc	0.0003852	Paxs	483.81	Joback Method
dvisc	0.0002518	Paxs	533.54	Joback Method
dvisc	0.0001770	Paxs	583.27	Joback Method
dvisc	0.0001315	Paxs	633.00	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=R33167&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
mccvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpolar:	Non-polar retention indices
ripolar:	Polar retention indices

tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume

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