

Decyl 4-chlorobutanoate

Other names:	Butanoic acid, 4-chloro, decyl ester
Inchi:	InChI=1S/C14H27ClO2/c1-2-3-4-5-6-7-8-9-13-17-14(16)11-10-12-15/h2-13H2,1H3
InchiKey:	UKINZMHKTPAMTL-UHFFFAOYSA-N
Formula:	C14H27ClO2
SMILES:	CCCCCCCCCOC(=O)CCCCl
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
mcpvol	227.800	ml/mol	McGowan Method
pc	1534.26	kPa	Joback Method
rinpol	1811.00		NIST Webbook
rinpol	1809.00		NIST Webbook
rinpol	1802.00		NIST Webbook
rinpol	1809.00		NIST Webbook
rinpol	1812.00		NIST Webbook
rinpol	1796.00		NIST Webbook
tb	633.44	K	Joback Method
tc	806.19	K	Joback Method
tf	349.62	K	Joback Method
vc	0.892	m ³ /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/molxK	719.81	Joback Method
cpg	661.20	J/molxK	748.60	Joback Method
cpg	674.62	J/molxK	777.39	Joback Method
cpg	687.38	J/molxK	806.19	Joback Method
dvisc	0.0022752	Paxs	349.62	Joback Method
dvisc	0.0010865	Paxs	396.92	Joback Method
dvisc	0.0006073	Paxs	444.23	Joback Method
dvisc	0.0003797	Paxs	491.53	Joback Method
dvisc	0.0002578	Paxs	538.83	Joback Method
dvisc	0.0001863	Paxs	586.14	Joback Method
dvisc	0.0001413	Paxs	633.44	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=R28148&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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

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