

Octyl 4-chlorobutanoate

Other names:	Butanoic acid, 4-chloro, octyl ester
Inchi:	InChI=1S/C12H23ClO2/c1-2-3-4-5-6-7-11-15-12(14)9-8-10-13/h2-11H2,1H3
InchiKey:	JLYKWKRZFITWIT-UHFFFAOYSA-N
Formula:	C12H23ClO2
SMILES:	CCCCCCCCOC(=O)CCCCl
Mol. weight [g/mol]:	234.76

Physical Properties

Property code	Value	Unit	Source
gf	-195.69	kJ/mol	Joback Method
hf	-551.55	kJ/mol	Joback Method
hfus	33.82	kJ/mol	Joback Method
hvap	55.85	kJ/mol	Joback Method
log10ws	-3.86		Crippen Method
logp	3.909		Crippen Method
mcvol	199.620	ml/mol	McGowan Method
pc	1793.94	kPa	Joback Method
rinpol	1607.00		NIST Webbook
rinpol	1601.00		NIST Webbook
rinpol	1599.00		NIST Webbook
rinpol	1611.00		NIST Webbook
rinpol	1605.00		NIST Webbook
rinpol	1619.00		NIST Webbook
rinpol	1605.00		NIST Webbook
rinpol	1619.00		NIST Webbook
tb	587.68	K	Joback Method
tc	762.26	K	Joback Method
tf	327.08	K	Joback Method
vc	0.780	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	496.42	J/mol×K	587.68	Joback Method

cpg	511.47	J/mol×K	616.78	Joback Method
cpg	525.87	J/mol×K	645.87	Joback Method
cpg	539.64	J/mol×K	674.97	Joback Method
cpg	552.80	J/mol×K	704.07	Joback Method
cpg	565.36	J/mol×K	733.17	Joback Method
cpg	577.32	J/mol×K	762.26	Joback Method
dvisc	0.0026085	Pa×s	327.08	Joback Method
dvisc	0.0012830	Pa×s	370.51	Joback Method
dvisc	0.0007323	Pa×s	413.95	Joback Method
dvisc	0.0004650	Pa×s	457.38	Joback Method
dvisc	0.0003194	Pa×s	500.81	Joback Method
dvisc	0.0002330	Pa×s	544.25	Joback Method
dvisc	0.0001781	Pa×s	587.68	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R28380&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

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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