

Propanoic acid, 2-chloro, octyl ester

Other names:	Octyl 2-chloropropanoate
Inchi:	InChI=1S/C11H21ClO2/c1-3-4-5-6-7-8-9-14-11(13)10(2)12/h10H,3-9H2,1-2H3
InchiKey:	BGMYZVCAOVIPM-UHFFFAOYSA-N
Formula:	C11H21ClO2
SMILES:	CCCCCCCCOC(=O)C(C)Cl
Mol. weight [g/mol]:	220.74

Physical Properties

Property code	Value	Unit	Source
gf	-206.55	kJ/mol	Joback Method
hf	-536.19	kJ/mol	Joback Method
hfus	27.71	kJ/mol	Joback Method
hvap	53.23	kJ/mol	Joback Method
log10ws	-3.55		Crippen Method
logp	3.517		Crippen Method
mcvol	185.530	ml/mol	McGowan Method
pc	1963.07	kPa	Joback Method
rinpol	1415.00		NIST Webbook
rinpol	1434.00		NIST Webbook
rinpol	1427.00		NIST Webbook
rinpol	1418.00		NIST Webbook
rinpol	1423.00		NIST Webbook
rinpol	1423.00		NIST Webbook
rinpol	1422.00		NIST Webbook
rinpol	1421.00		NIST Webbook
rinpol	1415.00		NIST Webbook
ripol	1772.00		NIST Webbook
ripol	1817.00		NIST Webbook
ripol	1787.00		NIST Webbook
ripol	1858.00		NIST Webbook
ripol	1837.00		NIST Webbook
ripol	1820.00		NIST Webbook
ripol	1814.00		NIST Webbook
tb	564.36	K	Joback Method
tc	743.50	K	Joback Method
tf	300.81	K	Joback Method
vc	0.719	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	446.93	J/molxK	564.36	Joback Method
cpg	461.63	J/molxK	594.22	Joback Method
cpg	475.70	J/molxK	624.07	Joback Method
cpg	489.15	J/molxK	653.93	Joback Method
cpg	501.98	J/molxK	683.78	Joback Method
cpg	514.22	J/molxK	713.64	Joback Method
cpg	525.87	J/molxK	743.50	Joback Method
dvisc	0.0036823	Paxs	300.81	Joback Method
dvisc	0.0016303	Paxs	344.74	Joback Method
dvisc	0.0008677	Paxs	388.66	Joback Method
dvisc	0.0005249	Paxs	432.59	Joback Method
dvisc	0.0003484	Paxs	476.51	Joback Method
dvisc	0.0002478	Paxs	520.44	Joback Method
dvisc	0.0001859	Paxs	564.36	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R23540&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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