3-Chloropropionic acid, octyl ester

Other names: Propanoic acid, 3-chloro, octyl ester
Octyl 3-chloropropanoate
Inchi: InChI=1S/C11H21ClO2/c1-2-3-4-5-6-7-10-14-11(13)8-9-12/h2-10H2,1H3
InchiKey: APSFWUHAPFXKHS-UHFFFAOYSA-N
Formula: C11H21ClO2
SMILES: CCCCCCCCOC(=O)CCCl
Mol. weight [g/mol]: 220.74
CAS: 63505-50-0

Physical Properties

Property code	Value	Unit	Source
gf	-204.11	kJ/mol	Joback Method
hf	-530.91	kJ/mol	Joback Method
hfus	31.23	kJ/mol	Joback Method
hvap	53.62	kJ/mol	Joback Method
log10ws	-3.44		Crippen Method
logp	3.519		Crippen Method
mcvol	185.530	ml/mol	McGowan Method
pc	1949.23	kPa	Joback Method
rinpol	1495.00		NIST Webbook
rinpol	1502.00		NIST Webbook
rinpol	1487.00		NIST Webbook
rinpol	1504.00		NIST Webbook
rinpol	1486.00		NIST Webbook
rinpol	1491.00		NIST Webbook
rinpol	1494.00		NIST Webbook
rinpol	1494.00		NIST Webbook
ripol	1949.00		NIST Webbook
ripol	1993.00		NIST Webbook
ripol	1949.00		NIST Webbook
ripol	2012.00		NIST Webbook
ripol	1926.00		NIST Webbook
ripol	1993.00		NIST Webbook
ripol	1982.00		NIST Webbook
ripol	1973.00		NIST Webbook
ripol	1970.00		NIST Webbook
tb	564.80	K	Joback Method

tc	740.70	K	Joback Method
tf	315.81	K	Joback Method
vc	0.725	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	446.60	J/mol×K	564.80	Joback Method
cpg	460.98	J/mol×K	594.12	Joback Method
cpg	474.76	J/mol×K	623.43	Joback Method
cpg	487.95	J/mol×K	652.75	Joback Method
cpg	500.56	J/mol×K	682.07	Joback Method
cpg	512.59	J/mol×K	711.39	Joback Method
cpg	524.06	J/mol×K	740.70	Joback Method
dvisc	0.0027568	Pa×s	315.81	Joback Method
dvisc	0.0013779	Pa×s	357.31	Joback Method
dvisc	0.0007956	Pa×s	398.81	Joback Method
dvisc	0.0005095	Pa×s	440.30	Joback Method
dvisc	0.0003523	Pa×s	481.80	Joback Method
dvisc	0.0002583	Pa×s	523.30	Joback Method
dvisc	0.0001982	Pa×s	564.80	Joback Method

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C63505500&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
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