2- Chloropropionic acid, octadecyl ester

Other names: Propanoic acid, 2-chloro, octadecyl ester
Inchi: InChI=1S/C21H41ClO2/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-24-21(23)20(2)
InchiKey: YQCZLISEEYFBDQ-UHFFFAOYSA-N
Formula: C21H41ClO2
SMILES: CCCCCCCCCCCCCCCCCCOC(=O)C(C)Cl
Mol. weight [g/mol]: 361.00
CAS: 88104-31-8

Physical Properties

Property code	Value	Unit	Source
gf	-122.35	kJ/mol	Joback Method
hf	-742.59	kJ/mol	Joback Method
hfus	53.61	kJ/mol	Joback Method
hvap	75.49	kJ/mol	Joback Method
log10ws	-7.74		Crippen Method
logp	7.418		Crippen Method
mcvol	326.430	ml/mol	McGowan Method
pc	966.27	kPa	Joback Method
rinpol	2427.00		NIST Webbook
rinpol	2460.50		NIST Webbook
ripol	2824.00		NIST Webbook
tb	793.16	K	Joback Method
tc	974.19	K	Joback Method
tf	413.51	K	Joback Method
vc	1.278	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1005.53	J/mol×K	793.16	Joback Method
cpg	1024.93	J/mol×K	823.33	Joback Method
cpg	1043.31	J/mol×K	853.50	Joback Method
cpg	1060.71	J/mol×K	883.67	Joback Method
cpg	1077.14	J/mol×K	913.85	Joback Method

cpg	1092.65	J/mol×K	944.02	Joback Method
cpg	1107.26	J/mol×K	974.19	Joback Method
dvisc	0.0014045	Pa×s	413.51	Joback Method
dvisc	0.0005600	Pa×s	476.78	Joback Method
dvisc	0.0002769	Pa×s	540.06	Joback Method
dvisc	0.0001588	Pa×s	603.34	Joback Method
dvisc	0.0001012	Pa×s	666.61	Joback Method
dvisc	0.0000697	Pa×s	729.88	Joback Method
dvisc	0.0000509	Pa×s	793.16	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=C88104318&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

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