2- Chloropropionic acid, hexadecyl ester

Other names: Propanoic acid, 2-chloro, hexadecyl ester
Hexadecyl 2-chloropropanoate
Inchi: InChI=1S/C19H37ClO2/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-22-19(21)18(2)20/h18
InchiKey: UHVQFSUSOVXCEO-UHFFFAOYSA-N
Formula: C19H37ClO2
SMILES: CCCCCCCCCCCCCCCCOC(=O)C(C)Cl
Mol. weight [g/mol]: 332.95
CAS: 86711-81-1

Physical Properties

Property code	Value	Unit	Source
gf	-139.19	kJ/mol	Joback Method
hf	-701.31	kJ/mol	Joback Method
hfus	48.43	kJ/mol	Joback Method
hvap	71.04	kJ/mol	Joback Method
log10ws	-6.90		Crippen Method
logp	6.638		Crippen Method
mcvol	298.250	ml/mol	McGowan Method
pc	1092.82	kPa	Joback Method
rinpol	2239.00		NIST Webbook
rinpol	2233.00		NIST Webbook
rinpol	2237.00		NIST Webbook
rinpol	2234.00		NIST Webbook
rinpol	2243.30		NIST Webbook
rinpol	2231.00		NIST Webbook
rinpol	2223.00		NIST Webbook
ripol	2612.00		NIST Webbook
ripol	2627.00		NIST Webbook
ripol	2640.00		NIST Webbook
ripol	2650.00		NIST Webbook
tb	747.40	K	Joback Method
tc	924.01	K	Joback Method
tf	390.97	K	Joback Method
vc	1.167	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	884.74	J/mol×K	747.40	Joback Method
cpg	968.63	J/mol×K	894.57	Joback Method
cpg	953.60	J/mol×K	865.14	Joback Method
cpg	937.72	J/mol×K	835.70	Joback Method
cpg	920.97	J/mol×K	806.27	Joback Method
cpg	903.32	J/mol×K	776.83	Joback Method
cpg	982.84	J/mol×K	924.01	Joback Method
dvisc	0.0000678	Pa×s	747.40	Joback Method
dvisc	0.0000924	Pa×s	687.99	Joback Method
dvisc	0.0001335	Pa×s	628.59	Joback Method
dvisc	0.0002082	Pa×s	569.18	Joback Method
dvisc	0.0003602	Pa×s	509.78	Joback Method
dvisc	0.0007200	Pa×s	450.38	Joback Method
dvisc	0.0017764	Pa×s	390.97	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=C86711811&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