3-Chloropropionic acid, hexadecyl ester

Other names: Propanoic acid, 3-chloro, hexadecyl ester
Hexadecyl 3-chloropropanoate
Inchi: InChI=1S/C19H37ClO2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-18-22-19(21)16-17-20/h2-
InchiKey: HKMCSNOMIKTPRU-UHFFFAOYSA-N
Formula: C19H37ClO2
SMILES: CCCCCCCCCCCCCCCCOC(=O)CCCl
Mol. weight [g/mol]: 332.95
CAS: 53312-70-2

Physical Properties

Property code	Value	Unit	Source
gf	-136.75	kJ/mol	Joback Method
hf	-696.03	kJ/mol	Joback Method
hfus	51.95	kJ/mol	Joback Method
hvap	71.43	kJ/mol	Joback Method
log10ws	-6.79		Crippen Method
logp	6.640		Crippen Method
mcvol	298.250	ml/mol	McGowan Method
pc	1087.06	kPa	Joback Method
rinpol	2311.00		NIST Webbook
rinpol	2306.00		NIST Webbook
rinpol	2305.00		NIST Webbook
rinpol	2302.00		NIST Webbook
rinpol	2298.00		NIST Webbook
rinpol	2312.00		NIST Webbook
ripol	2814.00		NIST Webbook
ripol	2786.00		NIST Webbook
ripol	2804.00		NIST Webbook
tb	747.84	K	Joback Method
tc	923.13	K	Joback Method
tf	405.97	K	Joback Method
vc	1.173	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	884.28	J/mol×K	747.84	Joback Method
cpg	902.70	J/mol×K	777.05	Joback Method
cpg	920.22	J/mol×K	806.27	Joback Method
cpg	936.86	J/mol×K	835.48	Joback Method
cpg	952.65	J/mol×K	864.70	Joback Method
cpg	967.61	J/mol×K	893.91	Joback Method
cpg	981.77	J/mol×K	923.13	Joback Method
dvisc	0.0014368	Pa×s	405.97	Joback Method
dvisc	0.0006456	Pa×s	462.95	Joback Method
dvisc	0.0003456	Pa×s	519.93	Joback Method
dvisc	0.0002094	Pa×s	576.90	Joback Method
dvisc	0.0001388	Pa×s	633.88	Joback Method
dvisc	0.0000984	Pa×s	690.86	Joback Method
dvisc	0.0000736	Pa×s	747.84	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C53312702&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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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