Hexadecyl 4-chlorobutanoate

Other names: Butanoic acid, 4-chloro, hexadecyl ester
hexadecyl 4-chlorobutyrate
Inchi: InChI=1S/C20H39ClO2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-19-23-20(22)17-16-18-21/
InchiKey: AIPUZHUOTILFRS-UHFFFAOYSA-N
Formula: C20H39ClO2
SMILES: CCCCCCCCCCCCCCCCOC(=O)CCCCl
Mol. weight [g/mol]: 346.98
CAS: 68516-31-4

Physical Properties

Property code	Value	Unit	Source
gf	-128.33	kJ/mol	Joback Method
hf	-716.67	kJ/mol	Joback Method
hfus	54.54	kJ/mol	Joback Method
hvap	73.66	kJ/mol	Joback Method
log10ws	-7.21		Crippen Method
logp	7.030		Crippen Method
mcvol	312.340	ml/mol	McGowan Method
pc	1021.38	kPa	Joback Method
rinpol	2417.00		NIST Webbook
rinpol	2412.00		NIST Webbook
rinpol	2406.00		NIST Webbook
rinpol	2406.00		NIST Webbook
tb	770.72	K	Joback Method
tc	948.17	K	Joback Method
tf	417.24	K	Joback Method
vc	1.228	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	944.23	J/mol×K	770.72	Joback Method
cpg	963.08	J/mol×K	800.30	Joback Method
cpg	980.99	J/mol×K	829.87	Joback Method

cpg	997.98	J/mol×K	859.45	Joback Method
cpg	1014.07	J/mol×K	889.02	Joback Method
cpg	1029.30	J/mol×K	918.60	Joback Method
cpg	1043.68	J/mol×K	948.17	Joback Method
dvisc	0.0012902	Pa×s	417.24	Joback Method
dvisc	0.0005737	Pa×s	476.15	Joback Method
dvisc	0.0003049	Pa×s	535.07	Joback Method
dvisc	0.0001837	Pa×s	593.98	Joback Method
dvisc	0.0001213	Pa×s	652.89	Joback Method
dvisc	0.0000858	Pa×s	711.81	Joback Method
dvisc	0.0000640	Pa×s	770.72	Joback Method

Sources

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=C68516314&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume