6-Chlorohexadecanoic acid, methyl ester

Inchi: InChI=1S/C17H33ClO2/c1-3-4-5-6-7-8-9-10-13-16(18)14-11-12-15-17(19)20-2/h16H,3-15
InchiKey: ZBGOIQVKISVQQM-UHFFFAOYSA-N
Formula: C17H33ClO2
SMILES: CCCCCCCCCCC(Cl)CCCCC(=O)OC
Mol. weight [g/mol]: 304.90

Physical Properties

Property code	Value	Unit	Source
gf	-156.03	kJ/mol	Joback Method
hf	-660.03	kJ/mol	Joback Method
hfus	43.25	kJ/mol	Joback Method
hvap	66.59	kJ/mol	Joback Method
log10ws	-6.07		Crippen Method
logp	5.858		Crippen Method
mcvol	270.070	ml/mol	McGowan Method
pc	1245.97	kPa	Joback Method
rinpol	2097.00		NIST Webbook
rinpol	2097.00		NIST Webbook
rinpol	2097.00		NIST Webbook
ripol	2557.00		NIST Webbook
ripol	2560.00		NIST Webbook
ripol	2560.00		NIST Webbook
tb	701.64	K	Joback Method
tc	876.28	K	Joback Method
tf	368.43	K	Joback Method
vc	1.054	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	767.83	J/mol×K	701.64	Joback Method
cpg	785.61	J/mol×K	730.75	Joback Method
cpg	802.54	J/mol×K	759.85	Joback Method
cpg	818.65	J/mol×K	788.96	Joback Method

cpg	833.96	J/mol×K	818.07	Joback Method
cpg	848.48	J/mol×K	847.17	Joback Method
cpg	862.24	J/mol×K	876.28	Joback Method
dvisc	0.0022085	Pa×s	368.43	Joback Method
dvisc	0.0009117	Pa×s	423.97	Joback Method
dvisc	0.0004619	Pa×s	479.50	Joback Method
dvisc	0.0002695	Pa×s	535.03	Joback Method
dvisc	0.0001741	Pa×s	590.57	Joback Method
dvisc	0.0001212	Pa×s	646.11	Joback Method
dvisc	0.0000893	Pa×s	701.64	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=R309645&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