15-Chlorohexadecanoic acid, methyl ester

Inchi: InChI=1S/C17H33ClO2/c1-16(18)14-12-10-8-6-4-3-5-7-9-11-13-15-17(19)20-2/h16H,3-15
InchiKey: UNWYWEKZNIHYAR-UHFFFAOYSA-N
Formula: C17H33ClO2
SMILES: COC(=O)CCCCCCCCCCCCCC(C)Cl
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	2127.00		NIST Webbook
rinpol	2127.00		NIST Webbook
ripol	2619.00		NIST Webbook
ripol	2613.00		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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R309056&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