

5-Chlorohexadecanoic acid, methyl ester

Inchi: InChI=1S/C17H33ClO2/c1-3-4-5-6-7-8-9-10-11-13-16(18)14-12-15-17(19)20-2/h16H,3-15H
InchiKey: CGCSETUTGCPCPQ-UHFFFAOYSA-N
Formula: C17H33ClO2
SMILES: CCCCCCCCCCCC(Cl)CCCC(=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	2089.00		NIST Webbook
rinpol	2090.00		NIST Webbook
ripol	2544.00		NIST Webbook
ripol	2547.00		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	848.48	J/mol×K	847.17	Joback Method
cpg	833.96	J/mol×K	818.07	Joback Method
cpg	818.65	J/mol×K	788.96	Joback Method
cpg	802.54	J/mol×K	759.85	Joback Method
cpg	785.61	J/mol×K	730.75	Joback Method

cpg	862.24	J/mol×K	876.28	Joback Method
dvisc	0.0000893	Pa×s	701.64	Joback Method
dvisc	0.0001212	Pa×s	646.11	Joback Method
dvisc	0.0001741	Pa×s	590.57	Joback Method
dvisc	0.0002695	Pa×s	535.03	Joback Method
dvisc	0.0004619	Pa×s	479.50	Joback Method
dvisc	0.0009117	Pa×s	423.97	Joback Method
dvisc	0.0022085	Pa×s	368.43	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=R309516&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

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