

16-Chlorohexadecanoic acid, methyl ester

Inchi:	InChI=1S/C17H33ClO2/c1-20-17(19)15-13-11-9-7-5-3-2-4-6-8-10-12-14-16-18/h2-16H2,
InchiKey:	XVFHLEIBPMFPQR-UHFFFAOYSA-N
Formula:	C17H33ClO2
SMILES:	COC(=O)CCCCCCCCCCCCCCCCI
Mol. weight [g/mol]:	304.90

Physical Properties

Property code	Value	Unit	Source
gf	-153.59	kJ/mol	Joback Method
hf	-654.75	kJ/mol	Joback Method
hfus	46.77	kJ/mol	Joback Method
hvap	66.98	kJ/mol	Joback Method
log10ws	-5.95		Crippen Method
logp	5.860		Crippen Method
mcvol	270.070	ml/mol	McGowan Method
pc	1238.96	kPa	Joback Method
ripol	2181.00		NIST Webbook
ripol	2178.00		NIST Webbook
ripol	2181.00		NIST Webbook
ripol	2696.00		NIST Webbook
ripol	2691.00		NIST Webbook
ripol	2696.00		NIST Webbook
tb	702.08	K	Joback Method
tc	874.86	K	Joback Method
tf	383.43	K	Joback Method
vc	1.060	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	767.38	J/molxK	702.08	Joback Method
cpg	784.94	J/molxK	730.88	Joback Method
cpg	801.69	J/molxK	759.67	Joback Method
cpg	817.63	J/molxK	788.47	Joback Method

cpg	832.80	J/molxK	817.27	Joback Method
cpg	847.21	J/molxK	846.07	Joback Method
cpg	860.88	J/molxK	874.86	Joback Method
dvisc	0.0017567	Paxs	383.43	Joback Method
dvisc	0.0008072	Paxs	436.54	Joback Method
dvisc	0.0004391	Paxs	489.65	Joback Method
dvisc	0.0002691	Paxs	542.75	Joback Method
dvisc	0.0001799	Paxs	595.86	Joback Method
dvisc	0.0001285	Paxs	648.97	Joback Method
dvisc	0.0000966	Paxs	702.08	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R309096&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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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