4-Chloropentadecanoic acid, methyl ester

Inchi: InChI=1S/C16H31ClO2/c1-3-4-5-6-7-8-9-10-11-12-15(17)13-14-16(18)19-2/h15H,3-14H2
InchiKey: QERRSGQGOADTFI-UHFFFAOYSA-N
Formula: C16H31ClO2
SMILES: CCCCCCCCCCCC(Cl)CCC(=O)OC
Mol. weight [g/mol]: 290.87

Physical Properties

Property code	Value	Unit	Source
gf	-164.45	kJ/mol	Joback Method
hf	-639.39	kJ/mol	Joback Method
hfus	40.66	kJ/mol	Joback Method
hvap	64.36	kJ/mol	Joback Method
log10ws	-5.65		Crippen Method
logp	5.468		Crippen Method
mcvol	255.980	ml/mol	McGowan Method
pc	1334.91	kPa	Joback Method
rinpol	1983.00		NIST Webbook
ripol	2419.00		NIST Webbook
ripol	2419.00		NIST Webbook
tb	678.76	K	Joback Method
tc	853.20	K	Joback Method
tf	357.16	K	Joback Method
vc	0.999	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	711.02	J/mol×K	678.76	Joback Method
cpg	789.95	J/mol×K	824.12	Joback Method
cpg	775.70	J/mol×K	795.05	Joback Method
cpg	760.71	J/mol×K	765.98	Joback Method
cpg	744.94	J/mol×K	736.91	Joback Method
cpg	728.39	J/mol×K	707.83	Joback Method
cpg	803.46	J/mol×K	853.20	Joback Method

dvisc	0.0001020	Pa×s	678.76	Joback Method
dvisc	0.0001380	Pa×s	625.16	Joback Method
dvisc	0.0001977	Pa×s	571.56	Joback Method
dvisc	0.0003050	Pa×s	517.96	Joback Method
dvisc	0.0005200	Pa×s	464.36	Joback Method
dvisc	0.0010191	Pa×s	410.76	Joback Method
dvisc	0.0024442	Pa×s	357.16	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=R309432&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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