5-Chlorooctadecanoic acid, methyl ester

Inchi: InChI=1S/C19H37ClO2/c1-3-4-5-6-7-8-9-10-11-12-13-15-18(20)16-14-17-19(21)22-2/h18
InchiKey: HOZLYMXZDIJUFO-UHFFFAOYSA-N
Formula: C19H37ClO2
SMILES: CCCCCCCCCCCCCC(Cl)CCCC(=O)OC
Mol. weight [g/mol]: 332.95

Physical Properties

Property code	Value	Unit	Source
gf	-139.19	kJ/mol	Joback Method
hf	-701.31	kJ/mol	Joback Method
hfus	48.43	kJ/mol	Joback Method
hvap	71.04	kJ/mol	Joback Method
log10ws	-6.90		Crippen Method
logp	6.638		Crippen Method
mcvol	298.250	ml/mol	McGowan Method
pc	1092.82	kPa	Joback Method
rinpol	2298.00		NIST Webbook
rinpol	2289.00		NIST Webbook
ripol	2737.00		NIST Webbook
ripol	2753.00		NIST Webbook
tb	747.40	K	Joback Method
tc	924.01	K	Joback Method
tf	390.97	K	Joback Method
vc	1.167	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	884.74	J/mol×K	747.40	Joback Method
cpg	903.32	J/mol×K	776.83	Joback Method
cpg	920.97	J/mol×K	806.27	Joback Method
cpg	937.72	J/mol×K	835.70	Joback Method
cpg	953.60	J/mol×K	865.14	Joback Method
cpg	968.63	J/mol×K	894.57	Joback Method

cpg	982.84	J/mol×K	924.01	Joback Method
dvisc	0.0017764	Pa×s	390.97	Joback Method
dvisc	0.0007200	Pa×s	450.38	Joback Method
dvisc	0.0003602	Pa×s	509.78	Joback Method
dvisc	0.0002082	Pa×s	569.18	Joback Method
dvisc	0.0001335	Pa×s	628.59	Joback Method
dvisc	0.0000924	Pa×s	687.99	Joback Method
dvisc	0.0000678	Pa×s	747.40	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R309541&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

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