6-Chlorooctadecanoic acid, methyl ester

Inchi: InChI=1S/C19H37ClO2/c1-3-4-5-6-7-8-9-10-11-12-15-18(20)16-13-14-17-19(21)22-2/h18
InchiKey: KWWNQFYYGQTOIT-UHFFFAOYSA-N
Formula: C19H37ClO2
SMILES: CCCCCCCCCCCCC(Cl)CCCCC(=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	2309.00		NIST Webbook
rinpol	2305.00		NIST Webbook
rinpol	2309.00		NIST Webbook
ripol	2761.00		NIST Webbook
ripol	2743.00		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=R309665&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

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