

13-Chlorooctadecanoic acid, methyl ester

Inchi:	InChI=1S/C19H37ClO2/c1-3-4-12-15-18(20)16-13-10-8-6-5-7-9-11-14-17-19(21)22-2/h18
InchiKey:	INHPOYBQHKUWGJ-UHFFFAOYSA-N
Formula:	C19H37ClO2
SMILES:	CCCCC(Cl)CCCCCCCCCCCC(=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
ripol	2319.00		NIST Webbook
ripol	2319.00		NIST Webbook
ripol	2320.00		NIST Webbook
ripol	2775.00		NIST Webbook
ripol	2775.00		NIST Webbook
ripol	2765.00		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/molxK	747.40	Joback Method
cpg	903.32	J/molxK	776.83	Joback Method
cpg	920.97	J/molxK	806.27	Joback Method
cpg	937.72	J/molxK	835.70	Joback Method

cpg	953.60	J/molxK	865.14	Joback Method
cpg	968.63	J/molxK	894.57	Joback Method
cpg	982.84	J/molxK	924.01	Joback Method
dvisc	0.0017764	Paxs	390.97	Joback Method
dvisc	0.0007200	Paxs	450.38	Joback Method
dvisc	0.0003602	Paxs	509.78	Joback Method
dvisc	0.0002082	Paxs	569.18	Joback Method
dvisc	0.0001335	Paxs	628.59	Joback Method
dvisc	0.0000924	Paxs	687.99	Joback Method
dvisc	0.0000678	Paxs	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=R308959&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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