Methyl 2-chloroheptadecanoate

Other names: 2-Chloroheptadecanoic acid, methyl ester
Inchi: InChI=1S/C18H35ClO2/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17(19)18(20)21-2/h17H,
InchiKey: ZZHLIYKVBVITFY-UHFFFAOYSA-N
Formula: C18H35ClO2
SMILES: CCCCCCCCCCCCCCCC(Cl)C(=O)OC
Mol. weight [g/mol]: 318.92
CAS: 77877-99-7

Physical Properties

Property code	Value	Unit	Source
gf	-147.61	kJ/mol	Joback Method
hf	-680.67	kJ/mol	Joback Method
hfus	45.84	kJ/mol	Joback Method
hvap	68.81	kJ/mol	Joback Method
log10ws	-6.48		Crippen Method
logp	6.248		Crippen Method
mcvol	284.160	ml/mol	McGowan Method
pc	1165.63	kPa	Joback Method
rinpol	2163.00		NIST Webbook
rinpol	2157.00		NIST Webbook
ripol	2548.00		NIST Webbook
ripol	2557.00		NIST Webbook
tb	724.52	K	Joback Method
tc	899.87	K	Joback Method
tf	379.70	K	Joback Method
vc	1.111	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	825.77	J/mol×K	724.52	Joback Method
cpg	908.06	J/mol×K	870.64	Joback Method
cpg	893.27	J/mol×K	841.42	Joback Method
cpg	877.67	J/mol×K	812.19	Joback Method

cpg	861.23	J/mol×K	782.97	Joback Method
cpg	843.94	J/mol×K	753.74	Joback Method
cpg	922.05	J/mol×K	899.87	Joback Method
dvisc	0.0000780	Pa×s	724.52	Joback Method
dvisc	0.0001060	Pa×s	667.05	Joback Method
dvisc	0.0001527	Pa×s	609.58	Joback Method
dvisc	0.0002373	Pa×s	552.11	Joback Method
dvisc	0.0004087	Pa×s	494.64	Joback Method
dvisc	0.0008119	Pa×s	437.17	Joback Method
dvisc	0.0019853	Pa×s	379.70	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=C77877997&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