11-Chloroheptadecanoic acid, methyl ester

Inchi: InChI=1S/C18H35ClO2/c1-3-4-5-11-14-17(19)15-12-9-7-6-8-10-13-16-18(20)21-2/h17H,3
InchiKey: NIJDOTYAXKJNDV-UHFFFAOYSA-N
Formula: C18H35ClO2
SMILES: CCCCCCC(Cl)CCCCCCCCCC(=O)OC
Mol. weight [g/mol]: 318.92

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	2205.00		NIST Webbook
rinpol	2220.00		NIST Webbook
ripol	2661.00		NIST Webbook
ripol	2675.00		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=R308800&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