17-Chloroheptadecanoic acid, methyl ester

Inchi: InChI=1S/C18H35ClO2/c1-21-18(20)16-14-12-10-8-6-4-2-3-5-7-9-11-13-15-17-19/h2-17H
InchiKey: NFKAAEGODPHLKP-UHFFFAOYSA-N
Formula: C18H35ClO2
SMILES: COC(=O)CCCCCCCCCCCCCCCCCl
Mol. weight [g/mol]: 318.92

Physical Properties

Property code	Value	Unit	Source
gf	-145.17	kJ/mol	Joback Method
hf	-675.39	kJ/mol	Joback Method
hfus	49.36	kJ/mol	Joback Method
hvap	69.20	kJ/mol	Joback Method
log10ws	-6.37		Crippen Method
logp	6.250		Crippen Method
mcvol	284.160	ml/mol	McGowan Method
pc	1159.29	kPa	Joback Method
rinpol	2289.00		NIST Webbook
rinpol	2277.00		NIST Webbook
ripol	2787.00		NIST Webbook
ripol	2800.00		NIST Webbook
tb	724.96	K	Joback Method
tc	898.71	K	Joback Method
tf	394.70	K	Joback Method
vc	1.117	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	825.31	J/mol×K	724.96	Joback Method
cpg	906.90	J/mol×K	869.75	Joback Method
cpg	892.21	J/mol×K	840.79	Joback Method
cpg	876.73	J/mol×K	811.84	Joback Method
cpg	860.43	J/mol×K	782.88	Joback Method
cpg	843.30	J/mol×K	753.92	Joback Method

cpg	920.82	J/mol×K	898.71	Joback Method
dvisc	0.0000844	Pa×s	724.96	Joback Method
dvisc	0.0001127	Pa×s	669.92	Joback Method
dvisc	0.0001583	Pa×s	614.87	Joback Method
dvisc	0.0002378	Pa×s	559.83	Joback Method
dvisc	0.0003904	Pa×s	504.79	Joback Method
dvisc	0.0007235	Pa×s	449.74	Joback Method
dvisc	0.0015927	Pa×s	394.70	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R309110&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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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