

13-Chloroheptadecanoic acid, methyl ester

Inchi:	InChI=1S/C18H35ClO2/c1-3-4-14-17(19)15-12-10-8-6-5-7-9-11-13-16-18(20)21-2/h17H,
InchiKey:	FWJGJIZHRVIRLT-UHFFFAOYSA-N
Formula:	C18H35ClO2
SMILES:	CCCC(Cl)CCCCCCCCCCCC(=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	2222.00		NIST Webbook
rinpol	2210.00		NIST Webbook
ripol	2686.00		NIST Webbook
ripol	2668.00		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/molxK	724.52	Joback Method
cpg	843.94	J/molxK	753.74	Joback Method
cpg	861.23	J/molxK	782.97	Joback Method
cpg	877.67	J/molxK	812.19	Joback Method
cpg	893.27	J/molxK	841.42	Joback Method
cpg	908.06	J/molxK	870.64	Joback Method

cpg	922.05	J/molxK	899.87	Joback Method
dvisc	0.0019853	Paxs	379.70	Joback Method
dvisc	0.0008119	Paxs	437.17	Joback Method
dvisc	0.0004087	Paxs	494.64	Joback Method
dvisc	0.0002373	Paxs	552.11	Joback Method
dvisc	0.0001527	Paxs	609.58	Joback Method
dvisc	0.0001060	Paxs	667.05	Joback Method
dvisc	0.0000780	Paxs	724.52	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R308939&Units=SI

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
ripol:	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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