Nonanoic acid, 8-chlorooctyl ester

Inchi: InChI=1S/C17H33ClO2/c1-2-3-4-5-8-11-14-17(19)20-16-13-10-7-6-9-12-15-18/h2-16H2,1

InchiKey: APFJCMJBKSBOSO-UHFFFAOYSA-N

Formula: C17H33ClO2

SMILES: CCCCCCCCC(=O)OCCCCCCCCCl

Mol. weight [g/mol]: 304.90

Physical Properties

Property code	Value	Unit	Source
gf	-153.59	kJ/mol	Joback Method
hf	-654.75	kJ/mol	Joback Method
hfus	46.77	kJ/mol	Joback Method
hvap	66.98	kJ/mol	Joback Method
log10ws	-5.95		Crippen Method
logp	5.860		Crippen Method
mcvol	270.070	ml/mol	McGowan Method
pc	1238.96	kPa	Joback Method
rinpol	2199.00		NIST Webbook
rinpol	2199.00		NIST Webbook
tb	702.08	K	Joback Method
tc	874.86	K	Joback Method
tf	383.43	K	Joback Method
vc	1.060	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	767.38	J/mol×K	702.08	Joback Method
cpg	784.94	J/mol×K	730.88	Joback Method
cpg	801.69	J/mol×K	759.67	Joback Method
cpg	817.63	J/mol×K	788.47	Joback Method
cpg	832.80	J/mol×K	817.27	Joback Method
cpg	847.21	J/mol×K	846.07	Joback Method
cpg	860.88	J/mol×K	874.86	Joback Method
dvisc	0.0017567	Pa×s	383.43	Joback Method

dvisc	0.0008072	Pa×s	436.54	Joback Method
dvisc	0.0004391	Pa×s	489.65	Joback Method
dvisc	0.0002691	Pa×s	542.75	Joback Method
dvisc	0.0001799	Pa×s	595.86	Joback Method
dvisc	0.0001285	Pa×s	648.97	Joback Method
dvisc	0.0000966	Pa×s	702.08	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U360672&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume