Hexanoic acid, 3,5,5-trimethyl-, 8-chlorooctyl ester

Inchi: InChI=1S/C17H33ClO2/c1-15(14-17(2,3)4)13-16(19)20-12-10-8-6-5-7-9-11-18/h15H,5-14

InchiKey: YHNYVZKZNOIRKW-UHFFFAOYSA-N

Formula: C17H33ClO2

SMILES: CC(CC(=O)OCCCCCCCCCl)CC(C)(C)C

Mol. weight [g/mol]: 304.90

Physical Properties

Property code	Value	Unit	Source
gf	-153.19	kJ/mol	Joback Method
hf	-668.78	kJ/mol	Joback Method
hfus	35.83	kJ/mol	Joback Method
hvap	65.29	kJ/mol	Joback Method
log10ws	-5.47		Crippen Method
logp	5.571		Crippen Method
mcvol	270.070	ml/mol	McGowan Method
pc	1262.85	kPa	Joback Method
rinpol	2034.00		NIST Webbook
rinpol	2034.00		NIST Webbook
tb	698.41	K	Joback Method
tc	878.84	K	Joback Method
tf	370.85	K	Joback Method
vc	1.044	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	769.92	J/mol×K	698.41	Joback Method
cpg	851.79	J/mol×K	848.77	Joback Method
cpg	837.13	J/mol×K	818.70	Joback Method
cpg	821.65	J/mol×K	788.63	Joback Method
cpg	805.31	J/mol×K	758.55	Joback Method
cpg	788.08	J/mol×K	728.48	Joback Method
cpg	865.65	J/mol×K	878.84	Joback Method
dvisc	0.0000751	Pa×s	698.41	Joback Method

dvisc	0.0001046	Pa×s	643.82	Joback Method
dvisc	0.0001550	Pa×s	589.22	Joback Method
dvisc	0.0002487	Pa×s	534.63	Joback Method
dvisc	0.0004444	Pa×s	480.04	Joback Method
dvisc	0.0009217	Pa×s	425.44	Joback Method
dvisc	0.0023699	Pa×s	370.85	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=U406828&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