Hexanoic acid, 3,5,5-trimethyl-, 2,2-dichloroethyl ester

Inchi: InChI=1S/C11H20Cl2O2/c1-8(6-11(2,3)4)5-10(14)15-7-9(12)13/h8-9H,5-7H2,1-4H3
InchiKey: RSKTUVAAPJFFDM-UHFFFAOYSA-N
Formula: C11H20Cl2O2
SMILES: CC(CC(=O)OCC(Cl)Cl)CC(C)(C)C
Mol. weight [g/mol]: 255.18

Physical Properties

Property code	Value	Unit	Source
gf	-218.08	kJ/mol	Joback Method
hf	-565.96	kJ/mol	Joback Method
hfus	20.97	kJ/mol	Joback Method
hvap	55.93	kJ/mol	Joback Method
log10ws	-3.72		Crippen Method
logp	3.796		Crippen Method
mcvol	197.770	ml/mol	McGowan Method
pc	1945.79	kPa	Joback Method
rinpol	1464.00		NIST Webbook
rinpol	1464.00		NIST Webbook
tb	598.12	K	Joback Method
tc	795.12	K	Joback Method
tf	318.15	K	Joback Method
vc	0.750	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	480.40	J/mol×K	598.12	Joback Method
cpg	495.41	J/mol×K	630.95	Joback Method
cpg	509.57	J/mol×K	663.79	Joback Method
cpg	522.92	J/mol×K	696.62	Joback Method
cpg	535.49	J/mol×K	729.45	Joback Method
cpg	547.32	J/mol×K	762.29	Joback Method
cpg	558.43	J/mol×K	795.12	Joback Method
dvisc	0.0047182	Pa×s	318.15	Joback Method

dvisc	0.0018172	Pa×s	364.81	Joback Method
dvisc	0.0008690	Pa×s	411.47	Joback Method
dvisc	0.0004829	Pa×s	458.13	Joback Method
dvisc	0.0002992	Pa×s	504.80	Joback Method
dvisc	0.0002010	Pa×s	551.46	Joback Method
dvisc	0.0001437	Pa×s	598.12	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=U406819&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume