Hexanoic acid, 3,5,5-trimethyl-, 3-chlorophenyl ester

Inchi: InChI=1S/C15H21ClO2/c1-11(10-15(2,3)4)8-14(17)18-13-7-5-6-12(16)9-13/h5-7,9,11H,8

InchiKey: MNAZLQAHROGLQR-UHFFFAOYSA-N

Formula: C15H21ClO2

SMILES: CC(CC(=O)Oc1cccc(Cl)c1)CC(C)(C)C

Mol. weight [g/mol]: 268.78

Physical Properties

Property code	Value	Unit	Source
gf	-67.25	kJ/mol	Joback Method
hf	-402.44	kJ/mol	Joback Method
hfus	24.30	kJ/mol	Joback Method
hvap	63.78	kJ/mol	Joback Method
log10ws	-4.92		Crippen Method
logp	4.708		Crippen Method
mcvol	218.130	ml/mol	McGowan Method
pc	1880.53	kPa	Joback Method
rinpol	1777.00		NIST Webbook
rinpol	1777.00		NIST Webbook
tb	684.31	K	Joback Method
tc	900.50	K	Joback Method
tf	387.25	K	Joback Method
vc	0.824	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	578.85	J/mol×K	684.31	Joback Method
cpg	595.29	J/mol×K	720.34	Joback Method
cpg	610.62	J/mol×K	756.37	Joback Method
cpg	624.91	J/mol×K	792.40	Joback Method
cpg	638.20	J/mol×K	828.44	Joback Method
cpg	650.55	J/mol×K	864.47	Joback Method
cpg	662.00	J/mol×K	900.50	Joback Method
dvisc	0.0016499	Pa×s	387.25	Joback Method

dvisc	0.0007884	Pa×s	436.76	Joback Method
dvisc	0.0004378	Pa×s	486.27	Joback Method
dvisc	0.0002711	Pa×s	535.78	Joback Method
dvisc	0.0001820	Pa×s	585.29	Joback Method
dvisc	0.0001300	Pa×s	634.80	Joback Method
dvisc	0.0000975	Pa×s	684.31	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=U406825&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