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

Inchi: InChI=1S/C15H20Cl2O2/c1-10(9-15(2,3)4)8-13(18)19-12-7-5-6-11(16)14(12)17/h5-7,10H

InchiKey: GPORBFFXACEAEP-UHFFFAOYSA-N

Formula: C15H20Cl2O2

SMILES: CC(CC(=O)Oc1cccc(Cl)c1Cl)CC(C)(C)C

Mol. weight [g/mol]: 303.22

Physical Properties

Property code	Value	Unit	Source
gf	-88.81	kJ/mol	Joback Method
hf	-429.65	kJ/mol	Joback Method
hfus	28.11	kJ/mol	Joback Method
hvap	68.83	kJ/mol	Joback Method
log10ws	-5.60		Crippen Method
logp	5.361		Crippen Method
mcvol	230.370	ml/mol	McGowan Method
pc	1798.51	kPa	Joback Method
rinpol	1968.00		NIST Webbook
rinpol	1968.00		NIST Webbook
tb	726.72	K	Joback Method
tc	946.78	K	Joback Method
tf	429.69	K	Joback Method
vc	0.873	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	605.50	J/mol×K	726.72	Joback Method
cpg	620.55	J/mol×K	763.40	Joback Method
cpg	634.56	J/mol×K	800.07	Joback Method
cpg	647.56	J/mol×K	836.75	Joback Method
cpg	659.62	J/mol×K	873.43	Joback Method
cpg	670.78	J/mol×K	910.11	Joback Method
cpg	681.10	J/mol×K	946.78	Joback Method
dvisc	0.0010589	Pa×s	429.69	Joback Method

dvisc	0.0005609	Pa×s	479.19	Joback Method
dvisc	0.0003347	Pa×s	528.70	Joback Method
dvisc	0.0002181	Pa×s	578.21	Joback Method
dvisc	0.0001521	Pa×s	627.71	Joback Method
dvisc	0.0001118	Pa×s	677.22	Joback Method
dvisc	0.0000857	Pa×s	726.72	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U406827&Units=SI
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

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