6-Chlorohexanoic acid, 3,4-dichlorophenyl ester

Inchi: InChI=1S/C12H13Cl3O2/c13-7-3-1-2-4-12(16)17-9-5-6-10(14)11(15)8-9/h5-6,8H,1-4,7H2

InchiKey: IBFRHXSHKRZPDS-UHFFFAOYSA-N

Formula: C12H13Cl3O2

SMILES: O=C(CCCCCCl)Oc1ccc(Cl)c(Cl)c1

Mol. weight [g/mol]: 295.59

Physical Properties

Property code	Value	Unit	Source
gf	-126.40	kJ/mol	Joback Method
hf	-369.44	kJ/mol	Joback Method
hfus	35.48	kJ/mol	Joback Method
hvap	68.22	kJ/mol	Joback Method
log10ws	-4.98		Crippen Method
logp	4.698		Crippen Method
mcvol	200.340	ml/mol	McGowan Method
pc	2195.89	kPa	Joback Method
rinpol	2090.00		NIST Webbook
rinpol	2090.00		NIST Webbook
tb	699.18	K	Joback Method
tc	917.61	K	Joback Method
tf	438.38	K	Joback Method
vc	0.770	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	470.43	J/mol×K	699.18	Joback Method
cpg	482.35	J/mol×K	735.59	Joback Method
cpg	493.46	J/mol×K	771.99	Joback Method
cpg	503.80	J/mol×K	808.40	Joback Method
cpg	513.37	J/mol×K	844.80	Joback Method
cpg	522.21	J/mol×K	881.21	Joback Method
cpg	530.33	J/mol×K	917.61	Joback Method
dvisc	0.0009923	Pa×s	438.38	Joback Method

dvisc	0.0006241	Pa×s	481.85	Joback Method
dvisc	0.0004238	Pa×s	525.31	Joback Method
dvisc	0.0003054	Pa×s	568.78	Joback Method
dvisc	0.0002305	Pa×s	612.25	Joback Method
dvisc	0.0001806	Pa×s	655.71	Joback Method
dvisc	0.0001458	Pa×s	699.18	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U307624&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