Acetic acid, (4-chlorophenoxy)-, isohexyl ester

Inchi: InChI=1S/C14H19ClO3/c1-11(2)4-3-9-17-14(16)10-18-13-7-5-12(15)6-8-13/h5-8,11H,3-4
InchiKey: RYWXAVANZWBQKP-UHFFFAOYSA-N
Formula: C14H19ClO3
SMILES: CC(C)CCCOC(=O)COc1ccc(Cl)cc1
Mol. weight [g/mol]: 270.75

Physical Properties

Property code	Value	Unit	Source
gf	-183.51	kJ/mol	Joback Method
hf	-505.27	kJ/mol	Joback Method
hfus	30.32	kJ/mol	Joback Method
hvap	65.26	kJ/mol	Joback Method
log10ws	-3.83		Crippen Method
logp	3.698		Crippen Method
mcvol	209.910	ml/mol	McGowan Method
pc	1982.35	kPa	Joback Method
rinpol	2376.00		NIST Webbook
rinpol	2376.00		NIST Webbook
tb	687.08	K	Joback Method
tc	893.55	K	Joback Method
tf	395.79	K	Joback Method
vc	0.796	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	550.11	J/mol×K	687.08	Joback Method
cpg	616.63	J/mol×K	859.14	Joback Method
cpg	605.11	J/mol×K	824.73	Joback Method
cpg	592.71	J/mol×K	790.32	Joback Method
cpg	579.41	J/mol×K	755.90	Joback Method
cpg	565.22	J/mol×K	721.49	Joback Method
cpg	627.28	J/mol×K	893.55	Joback Method
dvisc	0.0001005	Pa×s	687.08	Joback Method

dvisc	0.0001298	Pa×s	638.53	Joback Method
dvisc	0.0001748	Pa×s	589.98	Joback Method
dvisc	0.0002483	Pa×s	541.43	Joback Method
dvisc	0.0003781	Pa×s	492.89	Joback Method
dvisc	0.0006310	Pa×s	444.34	Joback Method
dvisc	0.0011940	Pa×s	395.79	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=U415098&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