Succinic acid, 2-chloropropyl isohexyl ester

Inchi: InChI=1S/C13H23ClO4/c1-10(2)5-4-8-17-12(15)6-7-13(16)18-9-11(3)14/h10-11H,4-9H2,
InchiKey: WCTQPSDQUVPTMD-UHFFFAOYSA-N
Formula: C13H23ClO4
SMILES: CC(C)CCCOC(=O)CCC(=O)OCC(C)Cl
Mol. weight [g/mol]: 278.77

Physical Properties

Property code	Value	Unit	Source
gf	-426.07	kJ/mol	Joback Method
hf	-827.55	kJ/mol	Joback Method
hfus	32.15	kJ/mol	Joback Method
hvap	66.45	kJ/mol	Joback Method
log10ws	-3.01		Crippen Method
logp	2.916		Crippen Method
mcvol	221.150	ml/mol	McGowan Method
pc	1743.37	kPa	Joback Method
rinpol	1799.00		NIST Webbook
rinpol	1799.00		NIST Webbook
tb	685.97	K	Joback Method
tc	872.11	K	Joback Method
tf	380.51	K	Joback Method
vc	0.849	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	599.34	J/mol×K	685.97	Joback Method
cpg	614.16	J/mol×K	716.99	Joback Method
cpg	628.21	J/mol×K	748.02	Joback Method
cpg	641.50	J/mol×K	779.04	Joback Method
cpg	654.03	J/mol×K	810.06	Joback Method
cpg	665.80	J/mol×K	841.09	Joback Method
cpg	676.82	J/mol×K	872.11	Joback Method
dvisc	0.0019951	Pa×s	380.51	Joback Method

dvisc	0.0009137	Pa×s	431.42	Joback Method
dvisc	0.0004935	Pa×s	482.33	Joback Method
dvisc	0.0002998	Pa×s	533.24	Joback Method
dvisc	0.0001986	Pa×s	584.15	Joback Method
dvisc	0.0001406	Pa×s	635.06	Joback Method
dvisc	0.0001048	Pa×s	685.97	Joback Method

Sources

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=U349372&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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