Succinic acid, monochloride 3-hexyl ester

Inchi: InChI=1S/C10H17ClO3/c1-3-5-8(4-2)14-10(13)7-6-9(11)12/h8H,3-7H2,1-2H3
InchiKey: YBFFUKFZMKXXSD-UHFFFAOYSA-N
Formula: C10H17ClO3
SMILES: CCCC(CC)OC(=O)CCC(=O)Cl
Mol. weight [g/mol]: 220.69

Physical Properties

Property code	Value	Unit	Source
gf	-343.89	kJ/mol	Joback Method
hf	-628.13	kJ/mol	Joback Method
hfus	26.72	kJ/mol	Joback Method
hvap	57.75	kJ/mol	Joback Method
log10ws	-2.91		Crippen Method
logp	2.654		Crippen Method
mcvol	173.010	ml/mol	McGowan Method
pc	2271.90	kPa	Joback Method
rinpol	1392.00		NIST Webbook
rinpol	1392.00		NIST Webbook
tb	595.35	K	Joback Method
tc	784.22	K	Joback Method
tf	339.47	K	Joback Method
vc	0.668	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	418.71	J/mol×K	595.35	Joback Method
cpg	431.70	J/mol×K	626.83	Joback Method
cpg	444.07	J/mol×K	658.31	Joback Method
cpg	455.83	J/mol×K	689.79	Joback Method
cpg	466.98	J/mol×K	721.27	Joback Method
cpg	477.53	J/mol×K	752.74	Joback Method
cpg	487.50	J/mol×K	784.22	Joback Method
dvisc	0.0029181	Pa×s	339.47	Joback Method

dvisc	0.0014748	Pa×s	382.12	Joback Method
dvisc	0.0008548	Pa×s	424.76	Joback Method
dvisc	0.0005473	Pa×s	467.41	Joback Method
dvisc	0.0003776	Pa×s	510.06	Joback Method
dvisc	0.0002758	Pa×s	552.70	Joback Method
dvisc	0.0002108	Pa×s	595.35	Joback Method

Sources

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=U349461&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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