Succinic acid, 2-chloro-5-methylphenyl hexyl ester

Inchi: InChI=1S/C17H23ClO4/c1-3-4-5-6-11-21-16(19)9-10-17(20)22-15-12-13(2)7-8-14(15)18/

InchiKey: ZBKODAUIOULRAU-UHFFFAOYSA-N

Formula: C17H23ClO4

SMILES: CCCCCCOC(=O)CCC(=O)Oc1cc(C)ccc1Cl

Mol. weight [g/mol]: 326.81

Physical Properties

Property code	Value	Unit	Source
gf	-294.36	kJ/mol	Joback Method
hf	-685.96	kJ/mol	Joback Method
hfus	42.82	kJ/mol	Joback Method
hvap	79.73	kJ/mol	Joback Method
log10ws	-5.16		Crippen Method
logp	4.458		Crippen Method
mcvol	253.750	ml/mol	McGowan Method
pc	1607.71	kPa	Joback Method
rinpol	2304.00		NIST Webbook
rinpol	2304.00		NIST Webbook
tb	815.01	K	Joback Method
tc	1020.37	K	Joback Method
tf	507.05	K	Joback Method
vc	0.977	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	730.36	J/mol×K	815.01	Joback Method
cpg	744.56	J/mol×K	849.24	Joback Method
cpg	757.73	J/mol×K	883.46	Joback Method
cpg	769.90	J/mol×K	917.69	Joback Method
cpg	781.06	J/mol×K	951.91	Joback Method
cpg	791.23	J/mol×K	986.14	Joback Method
cpg	800.43	J/mol×K	1020.37	Joback Method
dvisc	0.0005664	Pa×s	507.05	Joback Method

dvisc	0.0003441	Pa×s	558.38	Joback Method
dvisc	0.0002273	Pa×s	609.70	Joback Method
dvisc	0.0001601	Pa×s	661.03	Joback Method
dvisc	0.0001187	Pa×s	712.36	Joback Method
dvisc	0.0000915	Pa×s	763.68	Joback Method
dvisc	0.0000730	Pa×s	815.01	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=U353329&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