Succinic acid, 3-chlorophenyl 2-methylpent-3-yl ester

Inchi: InChI=1S/C16H21ClO4/c1-4-14(11(2)3)21-16(19)9-8-15(18)20-13-7-5-6-12(17)10-13/h5-

InchiKey: AUTCQRBOMFTBMB-UHFFFAOYSA-N

Formula: C16H21ClO4

SMILES: CCC(OC(=O)CCC(=O)Oc1cccc(Cl)c1)C(C)C

Mol. weight [g/mol]: 312.79

Physical Properties

Property code	Value	Unit	Source
gf	-298.03	kJ/mol	Joback Method
hf	-664.41	kJ/mol	Joback Method
hfus	33.57	kJ/mol	Joback Method
hvap	76.07	kJ/mol	Joback Method
log10ws	-4.55		Crippen Method
logp	4.003		Crippen Method
mcvol	239.660	ml/mol	McGowan Method
pc	1784.86	kPa	Joback Method
rinpol	2134.00		NIST Webbook
rinpol	2134.00		NIST Webbook
tb	786.27	K	Joback Method
tc	997.58	K	Joback Method
tf	453.26	K	Joback Method
vc	0.908	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	676.33	J/mol×K	786.27	Joback Method
cpg	690.72	J/mol×K	821.49	Joback Method
cpg	704.05	J/mol×K	856.71	Joback Method
cpg	716.33	J/mol×K	891.92	Joback Method
cpg	727.57	J/mol×K	927.14	Joback Method
cpg	737.79	J/mol×K	962.36	Joback Method
cpg	747.01	J/mol×K	997.58	Joback Method
dvisc	0.0009423	Pa×s	453.26	Joback Method

dvisc	0.0004823	Pa×s	508.76	Joback Method
dvisc	0.0002816	Pa×s	564.26	Joback Method
dvisc	0.0001811	Pa×s	619.76	Joback Method
dvisc	0.0001252	Pa×s	675.27	Joback Method
dvisc	0.0000916	Pa×s	730.77	Joback Method
dvisc	0.0000700	Pa×s	786.27	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=U389601&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