Succinic acid, 4-chloro-3-methylphenyl 3,3-dimethylbut-2-yl ester

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

InchiKey: DPASNZRHAYLTNB-UHFFFAOYSA-N

Formula: C17H23ClO4

SMILES: Cc1cc(OC(=O)CCC(=O)OC(C)C(C)(C)C)ccc1Cl

Mol. weight [g/mol]: 326.81

Physical Properties

Property code	Value	Unit	Source
gf	-293.96	kJ/mol	Joback Method
hf	-699.99	kJ/mol	Joback Method
hfus	31.88	kJ/mol	Joback Method
hvap	78.05	kJ/mol	Joback Method
log10ws	-5.03		Crippen Method
logp	4.312		Crippen Method
mcvol	253.750	ml/mol	McGowan Method
pc	1643.09	kPa	Joback Method
rinpol	2224.00		NIST Webbook
rinpol	2224.00		NIST Webbook
tb	811.34	K	Joback Method
tc	1026.92	K	Joback Method
tf	494.47	K	Joback Method
vc	0.960	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	732.46	J/mol×K	811.34	Joback Method
cpg	747.05	J/mol×K	847.27	Joback Method
cpg	760.53	J/mol×K	883.20	Joback Method
cpg	772.94	J/mol×K	919.13	Joback Method
cpg	784.29	J/mol×K	955.06	Joback Method
cpg	794.64	J/mol×K	990.99	Joback Method
cpg	804.01	J/mol×K	1026.92	Joback Method
dvisc	0.0005854	Pa×s	494.47	Joback Method

dvisc	0.0003242	Pa×s	547.28	Joback Method
dvisc	0.0001992	Pa×s	600.09	Joback Method
dvisc	0.0001324	Pa×s	652.90	Joback Method
dvisc	0.0000936	Pa×s	705.72	Joback Method
dvisc	0.0000694	Pa×s	758.53	Joback Method
dvisc	0.0000535	Pa×s	811.34	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=U390630&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