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

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

InchiKey: GNNLBHJAWGDKLM-UHFFFAOYSA-N

Formula: C17H23ClO4

SMILES: CCC(OC(=O)CCC(=O)Oc1ccc(Cl)cc1C)C(C)C

Mol. weight [g/mol]: 326.81

Physical Properties

Property code	Value	Unit	Source
gf	-299.24	kJ/mol	Joback Method
hf	-696.52	kJ/mol	Joback Method
hfus	35.77	kJ/mol	Joback Method
hvap	78.96	kJ/mol	Joback Method
log10ws	-5.03		Crippen Method
logp	4.312		Crippen Method
mcvol	253.750	ml/mol	McGowan Method
pc	1628.54	kPa	Joback Method
rinpol	2167.00		NIST Webbook
rinpol	2167.00		NIST Webbook
tb	814.13	K	Joback Method
tc	1024.57	K	Joback Method
tf	477.05	K	Joback Method
vc	0.965	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	731.48	J/mol×K	814.13	Joback Method
cpg	746.01	J/mol×K	849.20	Joback Method
cpg	759.44	J/mol×K	884.28	Joback Method
cpg	771.80	J/mol×K	919.35	Joback Method
cpg	783.08	J/mol×K	954.42	Joback Method
cpg	793.30	J/mol×K	989.50	Joback Method
cpg	802.47	J/mol×K	1024.57	Joback Method
dvisc	0.0007140	Pa×s	477.05	Joback Method

dvisc	0.0003826	Pa×s	533.23	Joback Method
dvisc	0.0002309	Pa×s	589.41	Joback Method
dvisc	0.0001521	Pa×s	645.59	Joback Method
dvisc	0.0001072	Pa×s	701.77	Joback Method
dvisc	0.0000795	Pa×s	757.95	Joback Method
dvisc	0.0000615	Pa×s	814.13	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=U390290&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