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

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

InchiKey: QUPDTWCKLOSRJN-UHFFFAOYSA-N

Formula: C16H21ClO4

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

Mol. weight [g/mol]: 312.79

Physical Properties

Property code	Value	Unit	Source
gf	-292.75	kJ/mol	Joback Method
hf	-667.88	kJ/mol	Joback Method
hfus	29.68	kJ/mol	Joback Method
hvap	75.16	kJ/mol	Joback Method
log10ws	-4.55		Crippen Method
logp	4.003		Crippen Method
mcvol	239.660	ml/mol	McGowan Method
pc	1801.56	kPa	Joback Method
rinpol	2079.00		NIST Webbook
rinpol	2079.00		NIST Webbook
tb	783.48	K	Joback Method
tc	1000.54	K	Joback Method
tf	470.68	K	Joback Method
vc	0.903	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	677.63	J/mol×K	783.48	Joback Method
cpg	692.10	J/mol×K	819.66	Joback Method
cpg	705.47	J/mol×K	855.83	Joback Method
cpg	717.77	J/mol×K	892.01	Joback Method
cpg	729.04	J/mol×K	928.18	Joback Method
cpg	739.33	J/mol×K	964.36	Joback Method
cpg	748.66	J/mol×K	1000.54	Joback Method
dvisc	0.0007742	Pa×s	470.68	Joback Method

dvisc	0.0004113	Pa×s	522.81	Joback Method
dvisc	0.0002451	Pa×s	574.95	Joback Method
dvisc	0.0001592	Pa×s	627.08	Joback Method
dvisc	0.0001104	Pa×s	679.21	Joback Method
dvisc	0.0000807	Pa×s	731.35	Joback Method
dvisc	0.0000615	Pa×s	783.48	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=U390628&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