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

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

InchiKey: BXKBMLLVFBPDGP-UHFFFAOYSA-N

Formula: C16H21ClO4

SMILES: Cc1ccc(OC(=O)CCC(=O)OC(C)C(C)C)c(Cl)c1

Mol. weight [g/mol]: 312.79

Physical Properties

Property code	Value	Unit	Source
gf	-307.66	kJ/mol	Joback Method
hf	-675.88	kJ/mol	Joback Method
hfus	33.18	kJ/mol	Joback Method
hvap	76.73	kJ/mol	Joback Method
log10ws	-4.61		Crippen Method
logp	3.922		Crippen Method
mcvol	239.660	ml/mol	McGowan Method
pc	1762.45	kPa	Joback Method
rinpol	2138.00		NIST Webbook
rinpol	2138.00		NIST Webbook
tb	791.25	K	Joback Method
tc	1003.34	K	Joback Method
tf	465.78	K	Joback Method
vc	0.908	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	675.30	J/mol×K	791.25	Joback Method
cpg	736.28	J/mol×K	967.99	Joback Method
cpg	726.17	J/mol×K	932.64	Joback Method
cpg	715.02	J/mol×K	897.30	Joback Method
cpg	702.84	J/mol×K	861.95	Joback Method
cpg	689.60	J/mol×K	826.60	Joback Method
cpg	745.38	J/mol×K	1003.34	Joback Method
dvisc	0.0000705	Pa×s	791.25	Joback Method

dvisc	0.0000908	Pa×s	737.00	Joback Method
dvisc	0.0001219	Pa×s	682.76	Joback Method
dvisc	0.0001722	Pa×s	628.51	Joback Method
dvisc	0.0002597	Pa×s	574.27	Joback Method
dvisc	0.0004265	Pa×s	520.02	Joback Method
dvisc	0.0007862	Pa×s	465.78	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=U390212&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