Succinic acid, 4-chloro-3-methylphenyl pent-4-en-2-yl ester

Inchi: InChI=1S/C16H19ClO4/c1-4-5-12(3)20-15(18)8-9-16(19)21-13-6-7-14(17)11(2)10-13/h4,

InchiKey: KGHVXEJBUKAHJP-UHFFFAOYSA-N

Formula: C16H19ClO4

SMILES: C=CCC(C)OC(=O)CCC(=O)Oc1ccc(Cl)c(C)c1

Mol. weight [g/mol]: 310.77

Physical Properties

Property code	Value	Unit	Source
gf	-217.38	kJ/mol	Joback Method
hf	-545.17	kJ/mol	Joback Method
hfus	35.43	kJ/mol	Joback Method
hvap	76.45	kJ/mol	Joback Method
log10ws	-4.70		Crippen Method
logp	3.842		Crippen Method
mcvol	235.360	ml/mol	McGowan Method
pc	1813.86	kPa	Joback Method
rinpol	2168.00		NIST Webbook
rinpol	2168.00		NIST Webbook
tb	788.37	K	Joback Method
tc	1000.33	K	Joback Method
tf	479.02	K	Joback Method
vc	0.895	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	648.86	J/mol×K	788.37	Joback Method
cpg	662.43	J/mol×K	823.70	Joback Method
cpg	675.00	J/mol×K	859.02	Joback Method
cpg	686.59	J/mol×K	894.35	Joback Method
cpg	697.20	J/mol×K	929.68	Joback Method
cpg	706.87	J/mol×K	965.00	Joback Method
cpg	715.59	J/mol×K	1000.33	Joback Method
dvisc	0.0007025	Pa×s	479.02	Joback Method

dvisc	0.0004122	Pa×s	530.58	Joback Method
dvisc	0.0002658	Pa×s	582.14	Joback Method
dvisc	0.0001841	Pa×s	633.69	Joback Method
dvisc	0.0001347	Pa×s	685.25	Joback Method
dvisc	0.0001030	Pa×s	736.81	Joback Method
dvisc	0.0000816	Pa×s	788.37	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=U391164&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