Succinic acid, 3-chlorophenyl pent-4-en-2-yl ester

Inchi: InChI=1S/C15H17ClO4/c1-3-5-11(2)19-14(17)8-9-15(18)20-13-7-4-6-12(16)10-13/h3-4,6

InchiKey: QFGZQDLIISJMCX-UHFFFAOYSA-N

Formula: C15H17ClO4

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

Mol. weight [g/mol]: 296.75

Physical Properties

Property code	Value	Unit	Source
gf	-216.17	kJ/mol	Joback Method
hf	-513.06	kJ/mol	Joback Method
hfus	33.23	kJ/mol	Joback Method
hvap	73.56	kJ/mol	Joback Method
log10ws	-4.23		Crippen Method
logp	3.533		Crippen Method
mcvol	221.270	ml/mol	McGowan Method
pc	1998.33	kPa	Joback Method
rinpol	2023.00		NIST Webbook
rinpol	2023.00		NIST Webbook
tb	760.51	K	Joback Method
tc	973.94	K	Joback Method
tf	455.23	K	Joback Method
vc	0.840	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	595.45	J/mol×K	760.51	Joback Method
cpg	652.56	J/mol×K	938.37	Joback Method
cpg	643.02	J/mol×K	902.80	Joback Method
cpg	632.56	J/mol×K	867.23	Joback Method
cpg	621.15	J/mol×K	831.65	Joback Method
cpg	608.79	J/mol×K	796.08	Joback Method
cpg	661.20	J/mol×K	973.94	Joback Method
dvisc	0.0000924	Pa×s	760.51	Joback Method

dvisc	0.0001179	Pa×s	709.63	Joback Method
dvisc	0.0001562	Pa×s	658.75	Joback Method
dvisc	0.0002170	Pa×s	607.87	Joback Method
dvisc	0.0003200	Pa×s	556.99	Joback Method
dvisc	0.0005103	Pa×s	506.11	Joback Method
dvisc	0.0009033	Pa×s	455.23	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=U391162&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