Succinic acid, 3-chlorophenyl cis-hex-2-en-1-yl ester

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

InchiKey: ZZBJJOKSNNAUSD-PLNGDYQASA-N

Formula: C16H19ClO4

SMILES: CCCC=CCOC(=O)CCC(=O)Oc1cccc(Cl)c1

Mol. weight [g/mol]: 310.77

Physical Properties

Property code	Value	Unit	Source
gf	-212.93	kJ/mol	Joback Method
hf	-536.63	kJ/mol	Joback Method
hfus	40.82	kJ/mol	Joback Method
hvap	76.80	kJ/mol	Joback Method
log10ws	-4.54		Crippen Method
logp	3.925		Crippen Method
mcvol	235.360	ml/mol	McGowan Method
pc	1840.41	kPa	Joback Method
rinpol	2254.00		NIST Webbook
rinpol	2254.00		NIST Webbook
tb	791.31	K	Joback Method
tc	1002.86	K	Joback Method
tf	478.18	K	Joback Method
vc	0.900	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	649.61	J/mol×K	791.31	Joback Method
cpg	663.09	J/mol×K	826.57	Joback Method
cpg	675.61	J/mol×K	861.83	Joback Method
cpg	687.19	J/mol×K	897.09	Joback Method
cpg	697.88	J/mol×K	932.35	Joback Method
cpg	707.68	J/mol×K	967.60	Joback Method
cpg	716.64	J/mol×K	1002.86	Joback Method
dvisc	0.0006625	Pa×s	478.18	Joback Method

dvisc	0.0003814	Pa×s	530.37	Joback Method
dvisc	0.0002424	Pa×s	582.56	Joback Method
dvisc	0.0001660	Pa×s	634.75	Joback Method
dvisc	0.0001204	Pa×s	686.93	Joback Method
dvisc	0.0000914	Pa×s	739.12	Joback Method
dvisc	0.0000719	Pa×s	791.31	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=U391305&Units=SI

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