Succinic acid, 3-chlorophenyl trans-hex-3-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/h3-

InchiKey: SQRAYFATJYUVQL-ONEGZZNKSA-N

Formula: C16H19ClO4

SMILES: CCC=CCCOC(=O)CCC(=O)Oc1cccc(Cl)c1

Mol. weight [g/mol]: 310.77

Physical Properties

Property code	Value	Unit	Source
hfus	43.98	kJ/mol	Joback Method
ie	8.63	eV	Cheméo Relay (1.0)
logp	3.925		Crippen Method
mcvol	235.360	ml/mol	McGowan Method
rinpol	2214.00		NIST Webbook
rinpol	2214.00		NIST Webbook
tb	619.39	K	Cheméo Relay (1.0)

Correlations

Information	Value
Property code	cpg
Equation	$Y = A + B \cdot T + C \cdot T^2 + D \cdot T^3 + E \cdot T.$
Y unit	J/mol×K
Coeff. A	1.82650e+01
Coeff. B	1.30262e+00
Coeff. C	-7.25760e-04
Coeff. D	1.22000e-07
Coeff. E	0.00000e+00
Basis	predicted
Temperature range (K), min.	273.00
Temperature range (K), max.	1000.00

Information	Value
Property code	dvisc

Equation	Y = exp(A + B/T + C·ln(T) + D·T^E)
Y unit	Pa×s
Coeff. A	-1.33909e+01
Coeff. B	2.72616e+03
Coeff. C	0.00000e+00
Coeff. D	0.00000e+00
Coeff. E	0.00000e+00
Basis	predicted
Comment	Liquid phase. Joback/Reid (1987), valid from Tf to 0.7·Tc.
Temperature range (K), min.	418.52
Temperature range (K), max.	674.09

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U391119&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
hfus:	Enthalpy of fusion at standard conditions
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature

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