Succinic acid, 2,3-dichlorophenyl cis-pent-2-en-1-yl ester

Inchi: InChI=1S/C15H16Cl2O4/c1-2-3-4-10-20-13(18)8-9-14(19)21-12-7-5-6-11(16)15(12)17/h3
InchiKey: QAFGCOMEZMFPCE-ARJAWSKDSA-N
Formula: C15H16Cl2O4
SMILES: CCC=CCOC(=O)CCC(=O)Oc1cccc(Cl)c1Cl
Mol. weight [g/mol]: 331.19

Physical Properties

Property code	Value	Unit	Source
hfus	45.20	kJ/mol	Joback Method
logp	4.188		Crippen Method
mcvol	233.510	ml/mol	McGowan Method
rinpol	2350.00		NIST Webbook
rinpol	2350.00		NIST Webbook

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	4.63640e+01
Coeff. B	1.15492e+00
Coeff. C	-6.24720e-04
Coeff. D	9.42000e-08
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	-1.33283e+01
Coeff. B	2.75206e+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.	449.69
Temperature range (K), max.	692.25

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
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=U391268&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

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

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