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

Inchi: InChI=1S/C15H16Cl2O4/c1-3-5-10(2)20-13(18)8-9-14(19)21-12-7-4-6-11(16)15(12)17/h3

InchiKey: LPAIOTXBAIHDPB-UHFFFAOYSA-N

Formula: C15H16Cl2O4

SMILES: C=CCC(C)OC(=O)CCC(=O)Oc1cccc(Cl)c1Cl

Mol. weight [g/mol]: 331.19

Physical Properties

Property code	Value	Unit	Source
gf	-237.73	kJ/mol	Joback Method
hf	-540.27	kJ/mol	Joback Method
hfus	37.03	kJ/mol	Joback Method
hvap	78.61	kJ/mol	Joback Method
log10ws	-4.91		Crippen Method
logp	4.187		Crippen Method
mcvol	233.510	ml/mol	McGowan Method
pc	1908.57	kPa	Joback Method
rinpol	2240.00		NIST Webbook
rinpol	2240.00		NIST Webbook
tb	802.92	K	Joback Method
tc	1020.39	K	Joback Method
tf	497.67	K	Joback Method
vc	0.888	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	617.95	J/mol×K	802.92	Joback Method
cpg	630.05	J/mol×K	839.16	Joback Method
cpg	641.18	J/mol×K	875.41	Joback Method
cpg	651.34	J/mol×K	911.65	Joback Method
cpg	660.56	J/mol×K	947.90	Joback Method
cpg	668.85	J/mol×K	984.14	Joback Method
cpg	676.23	J/mol×K	1020.39	Joback Method
dvisc	0.0006473	Pa×s	497.67	Joback Method

dvisc	0.0003909	Pa×s	548.54	Joback Method
dvisc	0.0002572	Pa×s	599.42	Joback Method
dvisc	0.0001807	Pa×s	650.29	Joback Method
dvisc	0.0001336	Pa×s	701.17	Joback Method
dvisc	0.0001029	Pa×s	752.04	Joback Method
dvisc	0.0000819	Pa×s	802.92	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=U391165&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