Succinic acid, 2,3-dichlorophenyl hept-1,6-dien-4-yl ester

Inchi: InChI=1S/C17H18Cl2O4/c1-3-6-12(7-4-2)22-15(20)10-11-16(21)23-14-9-5-8-13(18)17(14

InchiKey: LOEHMKZTOUAYQO-UHFFFAOYSA-N

Formula: C17H18Cl2O4

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

Mol. weight [g/mol]: 357.23

Physical Properties

Property code	Value	Unit	Source
gf	-133.05	kJ/mol	Joback Method
hf	-456.12	kJ/mol	Joback Method
hfus	40.93	kJ/mol	Joback Method
hvap	82.39	kJ/mol	Joback Method
log10ws	-5.60		Crippen Method
logp	4.743		Crippen Method
mcvol	257.390	ml/mol	McGowan Method
pc	1681.03	kPa	Joback Method
rinpol	2432.00		NIST Webbook
rinpol	2432.00		NIST Webbook
tb	845.36	K	Joback Method
tc	1061.92	K	Joback Method
tf	518.45	K	Joback Method
vc	0.982	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	701.68	J/mol×K	845.36	Joback Method
cpg	752.70	J/mol×K	1025.82	Joback Method
cpg	744.41	J/mol×K	989.73	Joback Method
cpg	735.19	J/mol×K	953.64	Joback Method
cpg	725.01	J/mol×K	917.55	Joback Method
cpg	713.85	J/mol×K	881.45	Joback Method
cpg	760.09	J/mol×K	1061.92	Joback Method
dvisc	0.0000665	Pa×s	845.36	Joback Method

dvisc	0.0000837	Pa×s	790.88	Joback Method
dvisc	0.0001091	Pa×s	736.39	Joback Method
dvisc	0.0001483	Pa×s	681.90	Joback Method
dvisc	0.0002126	Pa×s	627.42	Joback Method
dvisc	0.0003264	Pa×s	572.94	Joback Method
dvisc	0.0005484	Pa×s	518.45	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U391335&Units=SI
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

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