Succinic acid, 2,3-dichlorophenyl hex-5-en-1-yl ester

Inchi: InChI=1S/C16H18Cl2O4/c1-2-3-4-5-11-21-14(19)9-10-15(20)22-13-8-6-7-12(17)16(13)18

InchiKey: GXWIQODGOZWHDF-UHFFFAOYSA-N

Formula: C16H18Cl2O4

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

Mol. weight [g/mol]: 345.22

Physical Properties

Property code	Value	Unit	Source
gf	-226.87	kJ/mol	Joback Method
hf	-555.63	kJ/mol	Joback Method
hfus	43.15	kJ/mol	Joback Method
hvap	81.22	kJ/mol	Joback Method
log10ws	-5.22		Crippen Method
logp	4.578		Crippen Method
mcvol	247.600	ml/mol	McGowan Method
pc	1746.28	kPa	Joback Method
rinpol	2484.00		NIST Webbook
rinpol	2484.00		NIST Webbook
tb	826.24	K	Joback Method
tc	1038.96	K	Joback Method
tf	523.94	K	Joback Method
vc	0.951	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	672.27	J/mol×K	826.24	Joback Method
cpg	684.53	J/mol×K	861.69	Joback Method
cpg	695.82	J/mol×K	897.15	Joback Method
cpg	706.16	J/mol×K	932.60	Joback Method
cpg	715.56	J/mol×K	968.05	Joback Method
cpg	724.04	J/mol×K	1003.51	Joback Method
cpg	731.62	J/mol×K	1038.96	Joback Method
dvisc	0.0005360	Pa×s	523.94	Joback Method

dvisc	0.0003376	Pa×s	574.32	Joback Method
dvisc	0.0002290	Pa×s	624.71	Joback Method
dvisc	0.0001647	Pa×s	675.09	Joback Method
dvisc	0.0001239	Pa×s	725.47	Joback Method
dvisc	0.0000968	Pa×s	775.86	Joback Method
dvisc	0.0000779	Pa×s	826.24	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U391290&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