Succinic acid, dodec-2-en-1-yl 3-chlorophenyl ester

Inchi: InChI=1S/C22H31ClO4/c1-2-3-4-5-6-7-8-9-10-11-17-26-21(24)15-16-22(25)27-20-14-12-

InchiKey: SPGFJKZEHMWBTJ-ZHACJKMWSA-N

Formula: C22H31ClO4

SMILES: CCCCCCCCCC=CCOC(=O)CCC(=O)Oc1cccc(Cl)c1

Mol. weight [g/mol]: 394.93

Physical Properties

Property code	Value	Unit	Source
gf	-162.41	kJ/mol	Joback Method
hf	-660.47	kJ/mol	Joback Method
hfus	56.36	kJ/mol	Joback Method
hvap	90.16	kJ/mol	Joback Method
log10ws	-7.05		Crippen Method
logp	6.266		Crippen Method
mcvol	319.900	ml/mol	McGowan Method
pc	1183.34	kPa	Joback Method
rinpol	2896.00		NIST Webbook
rinpol	2896.00		NIST Webbook
tb	928.59	K	Joback Method
tc	1140.81	K	Joback Method
tf	545.80	K	Joback Method
vc	1.236	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	996.34	J/mol×K	928.59	Joback Method
cpg	1011.37	J/mol×K	963.96	Joback Method
cpg	1025.24	J/mol×K	999.33	Joback Method
cpg	1038.00	J/mol×K	1034.70	Joback Method
cpg	1049.70	J/mol×K	1070.07	Joback Method
cpg	1060.39	J/mol×K	1105.44	Joback Method
cpg	1070.12	J/mol×K	1140.81	Joback Method
dvisc	0.0003584	Pa×s	545.80	Joback Method

dvisc	0.0001922	Pa×s	609.60	Joback Method
dvisc	0.0001160	Pa×s	673.40	Joback Method
dvisc	0.0000764	Pa×s	737.19	Joback Method
dvisc	0.0000538	Pa×s	800.99	Joback Method
dvisc	0.0000399	Pa×s	864.79	Joback Method
dvisc	0.0000308	Pa×s	928.59	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U389859&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