Succinic acid, 4-chloro-3-methylphenyl hex-5-en-1-yl ester

Inchi: InChI=1S/C17H21ClO4/c1-3-4-5-6-11-21-16(19)9-10-17(20)22-14-7-8-15(18)13(2)12-14/

InchiKey: UPDFPDFCLIGDGL-UHFFFAOYSA-N

Formula: C17H21ClO4

SMILES: C=CCCCCOC(=O)CCC(=O)Oc1ccc(Cl)c(C)c1

Mol. weight [g/mol]: 324.80

Physical Properties

Property code	Value	Unit	Source
gf	-206.52	kJ/mol	Joback Method
hf	-560.53	kJ/mol	Joback Method
hfus	41.54	kJ/mol	Joback Method
hvap	79.06	kJ/mol	Joback Method
log10ws	-5.01		Crippen Method
logp	4.234		Crippen Method
mcvol	249.450	ml/mol	McGowan Method
pc	1663.26	kPa	Joback Method
rinpol	2420.00		NIST Webbook
rinpol	2420.00		NIST Webbook
tb	811.69	K	Joback Method
tc	1019.33	K	Joback Method
tf	505.29	K	Joback Method
vc	0.958	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	703.91	J/mol×K	811.69	Joback Method
cpg	717.59	J/mol×K	846.30	Joback Method
cpg	730.28	J/mol×K	880.90	Joback Method
cpg	741.99	J/mol×K	915.51	Joback Method
cpg	752.74	J/mol×K	950.11	Joback Method
cpg	762.54	J/mol×K	984.72	Joback Method
cpg	771.41	J/mol×K	1019.33	Joback Method
dvisc	0.0005783	Pa×s	505.29	Joback Method

dvisc	0.0003551	Pa×s	556.36	Joback Method
dvisc	0.0002367	Pa×s	607.42	Joback Method
dvisc	0.0001680	Pa×s	658.49	Joback Method
dvisc	0.0001253	Pa×s	709.56	Joback Method
dvisc	0.0000972	Pa×s	760.62	Joback Method
dvisc	0.0000778	Pa×s	811.69	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U391289&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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