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

Inchi: InChI=1S/C14H15ClO4/c1-2-3-9-18-13(16)7-8-14(17)19-12-6-4-5-11(15)10-12/h2-6,10H,

InchiKey: UFCQJKUWFCJQOX-NSCUHMNNSA-N

Formula: C14H15ClO4

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

Mol. weight [g/mol]: 282.72

Physical Properties

Property code	Value	Unit	Source
gf	-229.77	kJ/mol	Joback Method
hf	-495.35	kJ/mol	Joback Method
hfus	35.64	kJ/mol	Joback Method
hvap	72.35	kJ/mol	Joback Method
log10ws	-3.70		Crippen Method
logp	3.145		Crippen Method
mcvol	207.180	ml/mol	McGowan Method
pc	2185.64	kPa	Joback Method
rinpol	2059.00		NIST Webbook
rinpol	2059.00		NIST Webbook
tb	745.55	K	Joback Method
tc	961.97	K	Joback Method
tf	455.64	K	Joback Method
vc	0.788	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	541.42	J/mol×K	745.55	Joback Method
cpg	596.27	J/mol×K	925.90	Joback Method
cpg	587.01	J/mol×K	889.83	Joback Method
cpg	576.92	J/mol×K	853.76	Joback Method
cpg	565.98	J/mol×K	817.69	Joback Method
cpg	554.15	J/mol×K	781.62	Joback Method
cpg	604.71	J/mol×K	961.97	Joback Method
dvisc	0.0000932	Pa×s	745.55	Joback Method

dvisc	0.0001175	Pa×s	697.23	Joback Method
dvisc	0.0001534	Pa×s	648.91	Joback Method
dvisc	0.0002090	Pa×s	600.60	Joback Method
dvisc	0.0003005	Pa×s	552.28	Joback Method
dvisc	0.0004635	Pa×s	503.96	Joback Method
dvisc	0.0007834	Pa×s	455.64	Joback Method

Sources

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=U391226&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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