Succinic acid, 3-chlorophenyl but-3-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/h2,4-6,10

InchiKey: DYDQGOOQZXEJDS-UHFFFAOYSA-N

Formula: C14H15ClO4

SMILES: C=CCCOC(=O)CCC(=O)Oc1cccc(Cl)c1

Mol. weight [g/mol]: 282.72

Physical Properties

Property code	Value	Unit	Source
gf	-222.15	kJ/mol	Joback Method
hf	-487.14	kJ/mol	Joback Method
hfus	34.16	kJ/mol	Joback Method
hvap	71.72	kJ/mol	Joback Method
log10ws	-3.70		Crippen Method
logp	3.145		Crippen Method
mcvol	207.180	ml/mol	McGowan Method
pc	2165.35	kPa	Joback Method
rinpol	2016.00		NIST Webbook
rinpol	2016.00		NIST Webbook
tb	738.07	K	Joback Method
tc	950.72	K	Joback Method
tf	458.96	K	Joback Method
vc	0.789	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	541.43	J/mol×K	738.07	Joback Method
cpg	554.16	J/mol×K	773.51	Joback Method
cpg	565.98	J/mol×K	808.95	Joback Method
cpg	576.93	J/mol×K	844.40	Joback Method
cpg	586.99	J/mol×K	879.84	Joback Method
cpg	596.21	J/mol×K	915.28	Joback Method
cpg	604.57	J/mol×K	950.72	Joback Method
dvisc	0.0008600	Pa×s	458.96	Joback Method

dvisc	0.0005258	Pa×s	505.48	Joback Method
dvisc	0.0003493	Pa×s	552.00	Joback Method
dvisc	0.0002472	Pa×s	598.51	Joback Method
dvisc	0.0001840	Pa×s	645.03	Joback Method
dvisc	0.0001424	Pa×s	691.55	Joback Method
dvisc	0.0001139	Pa×s	738.07	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U391197&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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