Succinic acid, 4-chloro-3-methylphenyl but-2-en-1-yl ester

Inchi: InChI=1S/C15H17ClO4/c1-3-4-9-19-14(17)7-8-15(18)20-12-5-6-13(16)11(2)10-12/h3-6,1

InchiKey: RVRAUGUQRWCEGU-ONEGZZNKSA-N

Formula: C15H17ClO4

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

Mol. weight [g/mol]: 296.75

Physical Properties

Property code	Value	Unit	Source
gf	-230.98	kJ/mol	Joback Method
hf	-527.46	kJ/mol	Joback Method
hfus	37.84	kJ/mol	Joback Method
hvap	75.24	kJ/mol	Joback Method
log10ws	-4.17		Crippen Method
logp	3.453		Crippen Method
mcvol	221.270	ml/mol	McGowan Method
pc	1975.31	kPa	Joback Method
rinpol	2197.00		NIST Webbook
rinpol	2197.00		NIST Webbook
tb	773.41	K	Joback Method
tc	987.91	K	Joback Method
tf	479.43	K	Joback Method
vc	0.845	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	593.74	J/mol×K	773.41	Joback Method
cpg	649.94	J/mol×K	952.16	Joback Method
cpg	640.46	J/mol×K	916.41	Joback Method
cpg	630.12	J/mol×K	880.66	Joback Method
cpg	618.90	J/mol×K	844.91	Joback Method
cpg	606.78	J/mol×K	809.16	Joback Method
cpg	658.58	J/mol×K	987.91	Joback Method
dvisc	0.0000825	Pa×s	773.41	Joback Method

dvisc	0.0001030	Pa×s	724.41	Joback Method
dvisc	0.0001328	Pa×s	675.42	Joback Method
dvisc	0.0001782	Pa×s	626.42	Joback Method
dvisc	0.0002513	Pa×s	577.42	Joback Method
dvisc	0.0003777	Pa×s	528.43	Joback Method
dvisc	0.0006170	Pa×s	479.43	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=U391228&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