Succinic acid, 3-chlorophenyl 3-methylbut-3-en-1-yl ester

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

InchiKey: ZMEYPCVIZVHWCX-UHFFFAOYSA-N

Formula: C15H17ClO4

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

Mol. weight [g/mol]: 296.75

Physical Properties

Property code	Value	Unit	Source
gf	-222.28	kJ/mol	Joback Method
hf	-517.57	kJ/mol	Joback Method
hfus	35.44	kJ/mol	Joback Method
hvap	74.03	kJ/mol	Joback Method
log10ws	-4.12		Crippen Method
logp	3.535		Crippen Method
mcvol	221.270	ml/mol	McGowan Method
pc	1992.98	kPa	Joback Method
rinpol	2109.00		NIST Webbook
rinpol	2109.00		NIST Webbook
tb	760.83	K	Joback Method
tc	973.74	K	Joback Method
tf	456.27	K	Joback Method
vc	0.847	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	594.54	J/mol×K	760.83	Joback Method
cpg	607.82	J/mol×K	796.31	Joback Method
cpg	620.15	J/mol×K	831.80	Joback Method
cpg	631.54	J/mol×K	867.28	Joback Method
cpg	642.01	J/mol×K	902.77	Joback Method
cpg	651.59	J/mol×K	938.25	Joback Method
cpg	660.28	J/mol×K	973.74	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=U391140&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
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