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

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

InchiKey: WGXLXGARBQESNU-UHFFFAOYSA-N

Formula: C15H17ClO4

SMILES: CC(C)=CCOC(=O)CCC(=O)Oc1ccccc1Cl

Mol. weight [g/mol]: 296.75

Physical Properties

Property code	Value	Unit	Source
gf	-229.90	kJ/mol	Joback Method
hf	-525.78	kJ/mol	Joback Method
hfus	36.92	kJ/mol	Joback Method
hvap	74.66	kJ/mol	Joback Method
log10ws	-4.12		Crippen Method
logp	3.535		Crippen Method
mcvol	221.270	ml/mol	McGowan Method
pc	2010.90	kPa	Joback Method
rinpol	2129.00		NIST Webbook
rinpol	2129.00		NIST Webbook
tb	768.31	K	Joback Method
tc	984.84	K	Joback Method
tf	452.95	K	Joback Method
vc	0.846	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	594.63	J/mol×K	768.31	Joback Method
cpg	607.92	J/mol×K	804.40	Joback Method
cpg	620.26	J/mol×K	840.49	Joback Method
cpg	631.67	J/mol×K	876.58	Joback Method
cpg	642.18	J/mol×K	912.67	Joback Method
cpg	651.83	J/mol×K	948.75	Joback Method
cpg	660.63	J/mol×K	984.84	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=U389798&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