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

Inchi: InChI=1S/C16H19ClO4/c1-11(2)8-9-20-15(18)6-7-16(19)21-14-5-4-12(3)10-13(14)17/h4-

InchiKey: RSYRNPMUKHQPBL-UHFFFAOYSA-N

Formula: C16H19ClO4

SMILES: CC(C)=CCOC(=O)CCC(=O)Oc1ccc(C)cc1Cl

Mol. weight [g/mol]: 310.77

Physical Properties

Property code	Value	Unit	Source
gf	-231.11	kJ/mol	Joback Method
hf	-557.89	kJ/mol	Joback Method
hfus	39.12	kJ/mol	Joback Method
hvap	77.54	kJ/mol	Joback Method
log10ws	-4.59		Crippen Method
logp	3.843		Crippen Method
mcvol	235.360	ml/mol	McGowan Method
pc	1824.72	kPa	Joback Method
rinpol	2256.00		NIST Webbook
rinpol	2256.00		NIST Webbook
tb	796.17	K	Joback Method
tc	1011.06	K	Joback Method
tf	476.74	K	Joback Method
vc	0.901	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	648.10	J/mol×K	796.17	Joback Method
cpg	661.64	J/mol×K	831.98	Joback Method
cpg	674.22	J/mol×K	867.80	Joback Method
cpg	685.85	J/mol×K	903.61	Joback Method
cpg	696.55	J/mol×K	939.43	Joback Method
cpg	706.36	J/mol×K	975.24	Joback Method
cpg	715.30	J/mol×K	1011.06	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=U390214&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