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

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

InchiKey: VXHQNUYSKWQYQF-UHFFFAOYSA-N

Formula: C16H19ClO4

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

Mol. weight [g/mol]: 310.77

Physical Properties

Property code	Value	Unit	Source
gf	-223.49	kJ/mol	Joback Method
hf	-549.68	kJ/mol	Joback Method
hfus	37.64	kJ/mol	Joback Method
hvap	76.92	kJ/mol	Joback Method
log10ws	-4.59		Crippen Method
logp	3.843		Crippen Method
mcvol	235.360	ml/mol	McGowan Method
pc	1809.23	kPa	Joback Method
rinpol	2254.00		NIST Webbook
rinpol	2254.00		NIST Webbook
tb	788.69	K	Joback Method
tc	1000.18	K	Joback Method
tf	480.06	K	Joback Method
vc	0.902	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	647.93	J/mol×K	788.69	Joback Method
cpg	661.46	J/mol×K	823.94	Joback Method
cpg	674.01	J/mol×K	859.19	Joback Method
cpg	685.60	J/mol×K	894.43	Joback Method
cpg	696.25	J/mol×K	929.68	Joback Method
cpg	705.95	J/mol×K	964.93	Joback Method
cpg	714.75	J/mol×K	1000.18	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U391142&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

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