Succinic acid, 2,4,6-trichlorophenyl 3-methylbut-3-en-1-yl ester

Inchi: InChI=1S/C15H15Cl3O4/c1-9(2)5-6-21-13(19)3-4-14(20)22-15-11(17)7-10(16)8-12(15)18

InchiKey: WHCXJAWHCLQHMC-UHFFFAOYSA-N

Formula: C15H15Cl3O4

SMILES: C=C(C)CCOC(=O)CCC(=O)Oc1c(Cl)cc(Cl)cc1Cl

Mol. weight [g/mol]: 365.64

Physical Properties

Property code	Value	Unit	Source
gf	-265.40	kJ/mol	Joback Method
hf	-571.99	kJ/mol	Joback Method
hfus	43.05	kJ/mol	Joback Method
hvap	84.12	kJ/mol	Joback Method
log10ws	-5.49		Crippen Method
logp	4.842		Crippen Method
mcvol	245.750	ml/mol	McGowan Method
pc	1820.06	kPa	Joback Method
rinpol	2372.00		NIST Webbook
rinpol	2372.00		NIST Webbook
tb	845.65	K	Joback Method
tc	1066.73	K	Joback Method
tf	541.15	K	Joback Method
vc	0.945	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	637.43	J/mol×K	845.65	Joback Method
cpg	648.29	J/mol×K	882.50	Joback Method
cpg	658.21	J/mol×K	919.34	Joback Method
cpg	667.17	J/mol×K	956.19	Joback Method
cpg	675.20	J/mol×K	993.04	Joback Method
cpg	682.31	J/mol×K	1029.88	Joback Method
cpg	688.50	J/mol×K	1066.73	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U391145&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