Succinic acid, 3-methylbut-2-en-1-yl 2,4,6-trichlorophenyl 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: XHRSLDXMLPPRBE-UHFFFAOYSA-N

Formula: C15H15Cl3O4

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

Mol. weight [g/mol]: 365.64

Physical Properties

Property code	Value	Unit	Source
gf	-273.02	kJ/mol	Joback Method
hf	-580.20	kJ/mol	Joback Method
hfus	44.54	kJ/mol	Joback Method
hvap	84.75	kJ/mol	Joback Method
log10ws	-5.49		Crippen Method
logp	4.842		Crippen Method
mcvol	245.750	ml/mol	McGowan Method
pc	1835.69	kPa	Joback Method
rinpol	2352.00		NIST Webbook
rinpol	2352.00		NIST Webbook
tb	853.13	K	Joback Method
tc	1077.53	K	Joback Method
tf	537.83	K	Joback Method
vc	0.944	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	636.97	J/mol×K	853.13	Joback Method
cpg	647.88	J/mol×K	890.53	Joback Method
cpg	657.85	J/mol×K	927.93	Joback Method
cpg	666.93	J/mol×K	965.33	Joback Method
cpg	675.11	J/mol×K	1002.73	Joback Method
cpg	682.43	J/mol×K	1040.13	Joback Method
cpg	688.90	J/mol×K	1077.53	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U390272&Units=SI

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