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

Inchi: InChI=1S/C15H16Cl2O4/c1-10(2)8-9-20-13(18)6-7-14(19)21-12-5-3-4-11(16)15(12)17/h3

InchiKey: GHCDKYRPNNEKFQ-UHFFFAOYSA-N

Formula: C15H16Cl2O4

SMILES: C=C(C)CCOC(=O)CCC(=O)Oc1cccc(Cl)c1Cl

Mol. weight [g/mol]: 331.19

Physical Properties

Property code	Value	Unit	Source
gf	-243.84	kJ/mol	Joback Method
hf	-544.78	kJ/mol	Joback Method
hfus	39.25	kJ/mol	Joback Method
hvap	79.08	kJ/mol	Joback Method
log10ws	-4.80		Crippen Method
logp	4.188		Crippen Method
mcvol	233.510	ml/mol	McGowan Method
pc	1903.58	kPa	Joback Method
rinpol	2311.00		NIST Webbook
rinpol	2311.00		NIST Webbook
tb	803.24	K	Joback Method
tc	1020.21	K	Joback Method
tf	498.71	K	Joback Method
vc	0.895	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	617.01	J/mol×K	803.24	Joback Method
cpg	629.08	J/mol×K	839.40	Joback Method
cpg	640.19	J/mol×K	875.56	Joback Method
cpg	650.37	J/mol×K	911.73	Joback Method
cpg	659.63	J/mol×K	947.89	Joback Method
cpg	667.98	J/mol×K	984.05	Joback Method
cpg	675.45	J/mol×K	1020.21	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U391143&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