Succinic acid, 3-methylbut-2-en-1-yl 3,5-dichlorophenyl ester

Inchi: InChI=1S/C15H16Cl2O4/c1-10(2)5-6-20-14(18)3-4-15(19)21-13-8-11(16)7-12(17)9-13/h5

InchiKey: LWLGTUXBCVTZDT-UHFFFAOYSA-N

Formula: C15H16Cl2O4

SMILES: CC(C)=CCOC(=O)CCC(=O)Oc1cc(Cl)cc(Cl)c1

Mol. weight [g/mol]: 331.19

Physical Properties

Property code	Value	Unit	Source
gf	-251.46	kJ/mol	Joback Method
hf	-552.99	kJ/mol	Joback Method
hfus	40.73	kJ/mol	Joback Method
hvap	79.70	kJ/mol	Joback Method
log10ws	-4.80		Crippen Method
logp	4.188		Crippen Method
mcvol	233.510	ml/mol	McGowan Method
pc	1920.30	kPa	Joback Method
rinpol	2281.00		NIST Webbook
rinpol	2281.00		NIST Webbook
tb	810.72	K	Joback Method
tc	1031.17	K	Joback Method
tf	495.39	K	Joback Method
vc	0.894	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	616.80	J/mol×K	810.72	Joback Method
cpg	628.88	J/mol×K	847.46	Joback Method
cpg	640.03	J/mol×K	884.20	Joback Method
cpg	650.27	J/mol×K	920.94	Joback Method
cpg	659.61	J/mol×K	957.68	Joback Method
cpg	668.10	J/mol×K	994.43	Joback Method
cpg	675.75	J/mol×K	1031.17	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=U390147&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