Succinic acid, but-3-yn-2-yl 3,5-dichlorophenyl ester

Inchi: InChI=1S/C14H12Cl2O4/c1-3-9(2)19-13(17)4-5-14(18)20-12-7-10(15)6-11(16)8-12/h1,6-

InchiKey: VGEYTAIYMLOLHR-UHFFFAOYSA-N

Formula: C14H12Cl2O4

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

Mol. weight [g/mol]: 315.15

Physical Properties

Property code	Value	Unit	Source
gf	-110.92	kJ/mol	Joback Method
hf	-353.16	kJ/mol	Joback Method
hfus	38.70	kJ/mol	Joback Method
hvap	76.91	kJ/mol	Joback Method
log10ws	-4.44		Crippen Method
logp	3.244		Crippen Method
mcvol	215.120	ml/mol	McGowan Method
pc	2295.91	kPa	Joback Method
rinpol	2094.00		NIST Webbook
rinpol	2094.00		NIST Webbook
tb	773.48	K	Joback Method
tc	1001.77	K	Joback Method
tf	535.13	K	Joback Method
vc	0.814	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	538.07	J/mol×K	773.48	Joback Method
cpg	549.29	J/mol×K	811.53	Joback Method
cpg	559.57	J/mol×K	849.58	Joback Method
cpg	568.95	J/mol×K	887.62	Joback Method
cpg	577.42	J/mol×K	925.67	Joback Method
cpg	585.01	J/mol×K	963.72	Joback Method
cpg	591.72	J/mol×K	1001.77	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=U390144&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