Succinic acid, but-3-yn-2-yl 2,4,5-trichlorophenyl ester

Inchi: InChI=1S/C14H11Cl3O4/c1-3-8(2)20-13(18)4-5-14(19)21-12-7-10(16)9(15)6-11(12)17/h1

InchiKey: ZIEOGYZCTHAYCU-UHFFFAOYSA-N

Formula: C14H11Cl3O4

SMILES: C#CC(C)OC(=O)CCC(=O)Oc1cc(Cl)c(Cl)cc1Cl

Mol. weight [g/mol]: 349.59

Physical Properties

Property code	Value	Unit	Source
gf	-132.48	kJ/mol	Joback Method
hf	-380.37	kJ/mol	Joback Method
hfus	42.51	kJ/mol	Joback Method
hvap	81.96	kJ/mol	Joback Method
log10ws	-5.12		Crippen Method
logp	3.897		Crippen Method
mcvol	227.360	ml/mol	McGowan Method
pc	2185.64	kPa	Joback Method
rinpol	2211.00		NIST Webbook
rinpol	2211.00		NIST Webbook
tb	815.89	K	Joback Method
tc	1047.54	K	Joback Method
tf	577.57	K	Joback Method
vc	0.863	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	557.12	J/mol×K	815.89	Joback Method
cpg	567.13	J/mol×K	854.50	Joback Method
cpg	576.22	J/mol×K	893.11	Joback Method
cpg	584.40	J/mol×K	931.72	Joback Method
cpg	591.68	J/mol×K	970.33	Joback Method
cpg	598.06	J/mol×K	1008.94	Joback Method
cpg	603.55	J/mol×K	1047.54	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=U389961&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

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