Succinic acid, but-3-yn-2-yl 2,2,2-trichloroethyl ester

Inchi: InChI=1S/C10H11Cl3O4/c1-3-7(2)17-9(15)5-4-8(14)16-6-10(11,12)13/h1,7H,4-6H2,2H3

InchiKey: JORUEHRSAZFKGR-UHFFFAOYSA-N

Formula: C10H11Cl3O4

SMILES: C#CC(C)OC(=O)CCC(=O)OCC(Cl)(Cl)Cl

Mol. weight [g/mol]: 301.55

Physical Properties

Property code	Value	Unit	Source
gf	-246.84	kJ/mol	Joback Method
hf	-508.68	kJ/mol	Joback Method
hfus	31.86	kJ/mol	Joback Method
hvap	67.50	kJ/mol	Joback Method
log10ws	-3.20		Crippen Method
logp	2.245		Crippen Method
mcvol	194.760	ml/mol	McGowan Method
pc	2445.89	kPa	Joback Method
rinpol	1680.00		NIST Webbook
rinpol	1680.00		NIST Webbook
tb	679.52	K	Joback Method
tc	896.64	K	Joback Method
tf	470.93	K	Joback Method
vc	0.736	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	452.35	J/mol×K	679.52	Joback Method
cpg	462.61	J/mol×K	715.71	Joback Method
cpg	472.12	J/mol×K	751.89	Joback Method
cpg	480.91	J/mol×K	788.08	Joback Method
cpg	489.01	J/mol×K	824.26	Joback Method
cpg	496.44	J/mol×K	860.45	Joback Method
cpg	503.24	J/mol×K	896.64	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U390229&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

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