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

Inchi: InChI=1S/C10H12Cl2O4/c1-3-7(2)16-10(14)5-4-9(13)15-6-8(11)12/h1,7-8H,4-6H2,2H3
InchiKey: XFZHGSZTCPIFDY-UHFFFAOYSA-N
Formula: C10H12Cl2O4
SMILES: C#CC(C)OC(=O)CCC(=O)OCC(Cl)Cl
Mol. weight [g/mol]: 267.11

Physical Properties

Property code	Value	Unit	Source
gf	-240.19	kJ/mol	Joback Method
hf	-489.47	kJ/mol	Joback Method
hfus	31.55	kJ/mol	Joback Method
hvap	64.02	kJ/mol	Joback Method
log10ws	-2.55		Crippen Method
logp	1.678		Crippen Method
mcvol	182.520	ml/mol	McGowan Method
pc	2510.03	kPa	Joback Method
rinpol	1632.00		NIST Webbook
rinpol	1632.00		NIST Webbook
tb	644.88	K	Joback Method
tc	851.37	K	Joback Method
tf	423.59	K	Joback Method
vc	0.692	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	426.78	J/mol×K	644.88	Joback Method
cpg	437.82	J/mol×K	679.29	Joback Method
cpg	448.22	J/mol×K	713.71	Joback Method
cpg	457.97	J/mol×K	748.12	Joback Method
cpg	467.09	J/mol×K	782.54	Joback Method
cpg	475.58	J/mol×K	816.95	Joback Method
cpg	483.43	J/mol×K	851.37	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U390516&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