Succinic acid, but-3-yn-2-yl pent-4-en-2-yl ester

Inchi: InChI=1S/C13H18O4/c1-5-7-11(4)17-13(15)9-8-12(14)16-10(3)6-2/h2,5,10-11H,1,7-9H2,

InchiKey: KUFJFZLRNQIWDK-UHFFFAOYSA-N

Formula: C13H18O4

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

Mol. weight [g/mol]: 238.28

Physical Properties

Property code	Value	Unit	Source
gf	-103.23	kJ/mol	Joback Method
hf	-394.48	kJ/mol	Joback Method
hfus	29.65	kJ/mol	Joback Method
hvap	61.26	kJ/mol	Joback Method
log10ws	-2.86		Crippen Method
logp	1.839		Crippen Method
mcvol	196.010	ml/mol	McGowan Method
pc	2127.56	kPa	Joback Method
rinpol	1495.00		NIST Webbook
rinpol	1495.00		NIST Webbook
tb	635.34	K	Joback Method
tc	829.86	K	Joback Method
tf	395.80	K	Joback Method
vc	0.743	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	502.19	J/mol×K	635.34	Joback Method
cpg	516.24	J/mol×K	667.76	Joback Method
cpg	529.56	J/mol×K	700.18	Joback Method
cpg	542.16	J/mol×K	732.60	Joback Method
cpg	554.05	J/mol×K	765.02	Joback Method
cpg	565.24	J/mol×K	797.44	Joback Method
cpg	575.74	J/mol×K	829.86	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=U391152&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