Succinic acid, but-3-yn-2-yl cis-pent-2-en-1-yl ester

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

InchiKey: XMRSYNBCSDHMEZ-SREVYHEPSA-N

Formula: C13H18O4

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

Mol. weight [g/mol]: 238.28

Physical Properties

Property code	Value	Unit	Source
gf	-108.41	kJ/mol	Joback Method
hf	-397.41	kJ/mol	Joback Method
hfus	34.65	kJ/mol	Joback Method
hvap	62.27	kJ/mol	Joback Method
log10ws	-2.75		Crippen Method
logp	1.841		Crippen Method
mcvol	196.010	ml/mol	McGowan Method
pc	2131.49	kPa	Joback Method
rinpol	1591.00		NIST Webbook
rinpol	1591.00		NIST Webbook
tb	643.26	K	Joback Method
tc	838.20	K	Joback Method
tf	407.48	K	Joback Method
vc	0.748	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	502.36	J/mol×K	643.26	Joback Method
cpg	516.19	J/mol×K	675.75	Joback Method
cpg	529.29	J/mol×K	708.24	Joback Method
cpg	541.69	J/mol×K	740.73	Joback Method
cpg	553.40	J/mol×K	773.22	Joback Method
cpg	564.44	J/mol×K	805.71	Joback Method
cpg	574.82	J/mol×K	838.20	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=U391256&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