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

Inchi: InChI=1S/C13H18O4/c1-5-11(4)17-13(15)7-6-12(14)16-9-8-10(2)3/h1,11H,2,6-9H2,3-4H

InchiKey: GUJVOUIORAWIPO-UHFFFAOYSA-N

Formula: C13H18O4

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

Mol. weight [g/mol]: 238.28

Physical Properties

Property code	Value	Unit	Source
gf	-109.34	kJ/mol	Joback Method
hf	-398.99	kJ/mol	Joback Method
hfus	31.86	kJ/mol	Joback Method
hvap	61.72	kJ/mol	Joback Method
log10ws	-2.75		Crippen Method
logp	1.841		Crippen Method
mcvol	196.010	ml/mol	McGowan Method
pc	2121.68	kPa	Joback Method
rinpol	1566.00		NIST Webbook
rinpol	1566.00		NIST Webbook
tb	635.66	K	Joback Method
tc	829.65	K	Joback Method
tf	396.84	K	Joback Method
vc	0.750	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	501.46	J/mol×K	635.66	Joback Method
cpg	515.41	J/mol×K	667.99	Joback Method
cpg	528.64	J/mol×K	700.32	Joback Method
cpg	541.16	J/mol×K	732.65	Joback Method
cpg	552.99	J/mol×K	764.98	Joback Method
cpg	564.14	J/mol×K	797.32	Joback Method
cpg	574.61	J/mol×K	829.65	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U391131&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