Succinic acid, but-3-yn-2-yl hex-5-en-1-yl ester

Inchi: InChI=1S/C14H20O4/c1-4-6-7-8-11-17-13(15)9-10-14(16)18-12(3)5-2/h2,4,12H,1,6-11H2
InchiKey: UTGIIJOFKANWHB-UHFFFAOYSA-N
Formula: C14H20O4
SMILES: C#CC(C)OC(=O)CCC(=O)OCCCCC=C
Mol. weight [g/mol]: 252.31

Physical Properties

Property code	Value	Unit	Source
gf	-92.37	kJ/mol	Joback Method
hf	-409.84	kJ/mol	Joback Method
hfus	35.76	kJ/mol	Joback Method
hvap	63.87	kJ/mol	Joback Method
log10ws	-3.17		Crippen Method
logp	2.231		Crippen Method
mcvol	210.100	ml/mol	McGowan Method
pc	1937.24	kPa	Joback Method
rinpol	1680.00		NIST Webbook
rinpol	1680.00		NIST Webbook
tb	658.66	K	Joback Method
tc	847.95	K	Joback Method
tf	422.07	K	Joback Method
vc	0.804	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	553.15	J/mol×K	658.66	Joback Method
cpg	567.48	J/mol×K	690.21	Joback Method
cpg	581.08	J/mol×K	721.76	Joback Method
cpg	593.96	J/mol×K	753.31	Joback Method
cpg	606.12	J/mol×K	784.85	Joback Method
cpg	617.58	J/mol×K	816.40	Joback Method
cpg	628.35	J/mol×K	847.95	Joback Method

Sources

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=U391278&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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