Succinic acid, but-3-yn-2-yl 4-methylpent-2-yl ester

Inchi: InChI=1S/C14H22O4/c1-6-11(4)17-13(15)7-8-14(16)18-12(5)9-10(2)3/h1,10-12H,7-9H2,2

InchiKey: DVDTXJBVPTXCOA-UHFFFAOYSA-N

Formula: C14H22O4

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

Mol. weight [g/mol]: 254.32

Physical Properties

Property code	Value	Unit	Source
gf	-185.09	kJ/mol	Joback Method
hf	-545.83	kJ/mol	Joback Method
hfus	30.00	kJ/mol	Joback Method
hvap	63.76	kJ/mol	Joback Method
log10ws	-3.18		Crippen Method
logp	2.309		Crippen Method
mcvol	214.400	ml/mol	McGowan Method
pc	1893.65	kPa	Joback Method
rinpol	1528.00		NIST Webbook
rinpol	1528.00		NIST Webbook
tb	661.10	K	Joback Method
tc	853.68	K	Joback Method
tf	393.83	K	Joback Method
vc	0.811	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	576.87	J/mol×K	661.10	Joback Method
cpg	592.31	J/mol×K	693.20	Joback Method
cpg	606.96	J/mol×K	725.29	Joback Method
cpg	620.80	J/mol×K	757.39	Joback Method
cpg	633.86	J/mol×K	789.49	Joback Method
cpg	646.13	J/mol×K	821.58	Joback Method
cpg	657.64	J/mol×K	853.68	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U390423&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