Succinic acid, but-3-yn-2-yl 3,3-dimethylbut-2-yl ester

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

InchiKey: HXFUFCGOFAUJKX-UHFFFAOYSA-N

Formula: C14H22O4

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

Mol. weight [g/mol]: 254.32

Physical Properties

Property code	Value	Unit	Source
gf	-179.81	kJ/mol	Joback Method
hf	-549.30	kJ/mol	Joback Method
hfus	26.11	kJ/mol	Joback Method
hvap	62.86	kJ/mol	Joback Method
log10ws	-3.18		Crippen Method
logp	2.309		Crippen Method
mcvol	214.400	ml/mol	McGowan Method
pc	1911.91	kPa	Joback Method
rinpol	1531.00		NIST Webbook
rinpol	1531.00		NIST Webbook
tb	658.31	K	Joback Method
tc	856.92	K	Joback Method
tf	411.25	K	Joback Method
vc	0.806	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	579.23	J/mol×K	658.31	Joback Method
cpg	594.93	J/mol×K	691.41	Joback Method
cpg	609.73	J/mol×K	724.51	Joback Method
cpg	623.67	J/mol×K	757.61	Joback Method
cpg	636.75	J/mol×K	790.72	Joback Method
cpg	649.01	J/mol×K	823.82	Joback Method
cpg	660.48	J/mol×K	856.92	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=U390617&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