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

Inchi: InChI=1S/C13H18O5/c1-3-10(2)18-13(15)7-6-12(14)17-9-11-5-4-8-16-11/h1,10-11H,4-9H

InchiKey: GBPBBBUZPABQIG-UHFFFAOYSA-N

Formula: C13H18O5

SMILES: C#CC(C)OC(=O)CCC(=O)OCC1CCCO1

Mol. weight [g/mol]: 254.28

Physical Properties

Property code	Value	Unit	Source
gf	-238.20	kJ/mol	Joback Method
hf	-586.15	kJ/mol	Joback Method
hfus	36.37	kJ/mol	Joback Method
hvap	67.08	kJ/mol	Joback Method
log10ws	-1.99		Crippen Method
logp	1.054		Crippen Method
mcvol	195.320	ml/mol	McGowan Method
pc	2386.52	kPa	Joback Method
rinpol	1788.00		NIST Webbook
rinpol	1788.00		NIST Webbook
tb	681.33	K	Joback Method
tc	891.37	K	Joback Method
tf	450.03	K	Joback Method
vc	0.730	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	544.52	J/mol×K	681.33	Joback Method
cpg	559.98	J/mol×K	716.34	Joback Method
cpg	574.46	J/mol×K	751.34	Joback Method
cpg	587.99	J/mol×K	786.35	Joback Method
cpg	600.57	J/mol×K	821.35	Joback Method
cpg	612.23	J/mol×K	856.36	Joback Method
cpg	622.98	J/mol×K	891.37	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=U390713&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