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

Inchi: InChI=1S/C15H24O4/c1-7-12(6)18-13(16)8-9-14(17)19-15(10(2)3)11(4)5/h1,10-12,15H,8

InchiKey: HXFYVZAUYVGUKI-UHFFFAOYSA-N

Formula: C15H24O4

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

Mol. weight [g/mol]: 268.35

Physical Properties

Property code	Value	Unit	Source
gf	-179.11	kJ/mol	Joback Method
hf	-571.75	kJ/mol	Joback Method
hfus	29.06	kJ/mol	Joback Method
hvap	65.60	kJ/mol	Joback Method
log10ws	-3.36		Crippen Method
logp	2.555		Crippen Method
mcvol	228.490	ml/mol	McGowan Method
pc	1756.54	kPa	Joback Method
rinpol	1624.00		NIST Webbook
tb	683.54	K	Joback Method
tc	877.40	K	Joback Method
tf	390.10	K	Joback Method
vc	0.862	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	630.87	J/mol×K	683.54	Joback Method
cpg	647.05	J/mol×K	715.85	Joback Method
cpg	662.35	J/mol×K	748.16	Joback Method
cpg	676.77	J/mol×K	780.47	Joback Method
cpg	690.35	J/mol×K	812.78	Joback Method
cpg	703.07	J/mol×K	845.09	Joback Method
cpg	714.96	J/mol×K	877.40	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=U390501&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