Succinic acid, but-3-yn-2-yl 1-phenylpropyl ester

Inchi: InChI=1S/C17H20O4/c1-4-13(3)20-16(18)11-12-17(19)21-15(5-2)14-9-7-6-8-10-14/h1,6-

InchiKey: LCWZJIMASFNTAL-UHFFFAOYSA-N

Formula: C17H20O4

SMILES: C#CC(C)OC(=O)CCC(=O)OC(CC)c1ccccc1

Mol. weight [g/mol]: 288.34

Physical Properties

Property code	Value	Unit	Source
gf	-44.98	kJ/mol	Joback Method
hf	-365.94	kJ/mol	Joback Method
hfus	35.33	kJ/mol	Joback Method
hvap	73.11	kJ/mol	Joback Method
log10ws	-4.13		Crippen Method
logp	3.026		Crippen Method
mcvol	232.910	ml/mol	McGowan Method
pc	1952.68	kPa	Joback Method
rinpol	1923.00		NIST Webbook
rinpol	1923.00		NIST Webbook
tb	756.86	K	Joback Method
tc	971.95	K	Joback Method
tf	469.06	K	Joback Method
vc	0.877	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	654.34	J/mol×K	756.86	Joback Method
cpg	669.43	J/mol×K	792.71	Joback Method
cpg	683.43	J/mol×K	828.56	Joback Method
cpg	696.37	J/mol×K	864.40	Joback Method
cpg	708.28	J/mol×K	900.25	Joback Method
cpg	719.20	J/mol×K	936.10	Joback Method
cpg	729.15	J/mol×K	971.95	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=U389922&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