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

Inchi: InChI=1S/C17H20O5/c1-5-13(4)21-16(18)10-11-17(19)22-15-9-7-6-8-14(15)20-12(2)3/h1

InchiKey: NUKNIFPVDVNUCG-UHFFFAOYSA-N

Formula: C17H20O5

SMILES: C#CC(C)OC(=O)CCC(=O)Oc1ccccc1OC(C)C

Mol. weight [g/mol]: 304.34

Physical Properties

Property code	Value	Unit	Source
gf	-159.61	kJ/mol	Joback Method
hf	-509.63	kJ/mol	Joback Method
hfus	36.13	kJ/mol	Joback Method
hvap	76.18	kJ/mol	Joback Method
log10ws	-4.13		Crippen Method
logp	2.724		Crippen Method
mcvol	238.780	ml/mol	McGowan Method
pc	1898.60	kPa	Joback Method
rinpol	2032.00		NIST Webbook
rinpol	2032.00		NIST Webbook
tb	784.26	K	Joback Method
tc	998.50	K	Joback Method
tf	503.81	K	Joback Method
vc	0.895	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	680.62	J/mol×K	784.26	Joback Method
cpg	695.14	J/mol×K	819.97	Joback Method
cpg	708.56	J/mol×K	855.67	Joback Method
cpg	720.89	J/mol×K	891.38	Joback Method
cpg	732.13	J/mol×K	927.08	Joback Method
cpg	742.29	J/mol×K	962.79	Joback Method
cpg	751.38	J/mol×K	998.50	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U389786&Units=SI

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