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

Inchi: InChI=1S/C17H20O4/c1-4-8-14-9-6-7-10-15(14)21-17(19)12-11-16(18)20-13(3)5-2/h2,6-

InchiKey: LBYLTYXERNZXEO-UHFFFAOYSA-N

Formula: C17H20O4

SMILES: C#CC(C)OC(=O)CCC(=O)Oc1ccccc1CCC

Mol. weight [g/mol]: 288.34

Physical Properties

Property code	Value	Unit	Source
gf	-52.17	kJ/mol	Joback Method
hf	-372.13	kJ/mol	Joback Method
hfus	38.46	kJ/mol	Joback Method
hvap	74.16	kJ/mol	Joback Method
log10ws	-4.29		Crippen Method
logp	2.890		Crippen Method
mcvol	232.910	ml/mol	McGowan Method
pc	1913.58	kPa	Joback Method
rinpol	1946.00		NIST Webbook
rinpol	1946.00		NIST Webbook
tb	762.28	K	Joback Method
tc	974.80	K	Joback Method
tf	496.58	K	Joback Method
vc	0.883	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	652.83	J/mol×K	762.28	Joback Method
cpg	667.56	J/mol×K	797.70	Joback Method
cpg	681.27	J/mol×K	833.12	Joback Method
cpg	693.97	J/mol×K	868.54	Joback Method
cpg	705.69	J/mol×K	903.96	Joback Method
cpg	716.45	J/mol×K	939.38	Joback Method
cpg	726.28	J/mol×K	974.80	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=U390385&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