Succinic acid, hex-4-yn-3-yl 3-methoxyphenyl ester

Inchi: InChI=1S/C17H20O5/c1-4-7-13(5-2)21-16(18)10-11-17(19)22-15-9-6-8-14(12-15)20-3/h6
InchiKey: SXQSFMIWZUHTOM-UHFFFAOYSA-N
Formula: C17H20O5
SMILES: CC#CC(CC)OC(=O)CCC(=O)Oc1cccc(OC)c1
Mol. weight [g/mol]: 304.34

Physical Properties

Property code	Value	Unit	Source
gf	-177.44	kJ/mol	Joback Method
hf	-523.95	kJ/mol	Joback Method
hfus	39.80	kJ/mol	Joback Method
hvap	78.86	kJ/mol	Joback Method
log10ws	-4.02		Crippen Method
logp	2.726		Crippen Method
mcvol	238.780	ml/mol	McGowan Method
pc	1905.24	kPa	Joback Method
rinpol	2283.00		NIST Webbook
rinpol	2283.00		NIST Webbook
tb	803.58	K	Joback Method
tc	1022.27	K	Joback Method
tf	577.94	K	Joback Method
vc	0.901	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	683.16	J/mol×K	803.58	Joback Method
cpg	697.70	J/mol×K	840.03	Joback Method
cpg	711.09	J/mol×K	876.48	Joback Method
cpg	723.31	J/mol×K	912.92	Joback Method
cpg	734.36	J/mol×K	949.37	Joback Method
cpg	744.24	J/mol×K	985.82	Joback Method
cpg	752.94	J/mol×K	1022.27	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=U390980&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