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

Inchi: InChI=1S/C22H22O4/c1-3-8-19(4-2)25-21(23)15-16-22(24)26-20-13-11-18(12-14-20)17-
InchiKey: YNNYSZLVZDGNEV-UHFFFAOYSA-N
Formula: C22H22O4
SMILES: CC#CC(CC)OC(=O)CCC(=O)Oc1ccc(-c2ccccc2)cc1
Mol. weight [g/mol]: 350.41

Physical Properties

Property code	Value	Unit	Source
gf	82.07	kJ/mol	Joback Method
hf	-258.40	kJ/mol	Joback Method
hfus	45.60	kJ/mol	Joback Method
hvap	89.86	kJ/mol	Joback Method
log10ws	-6.51		Crippen Method
logp	4.384		Crippen Method
mcvol	279.600	ml/mol	McGowan Method
pc	1703.31	kPa	Joback Method
rinpol	2885.00		NIST Webbook
rinpol	2885.00		NIST Webbook
tb	922.24	K	Joback Method
tc	1161.46	K	Joback Method
tf	638.48	K	Joback Method
vc	1.056	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	843.23	J/mol×K	922.24	Joback Method
cpg	856.97	J/mol×K	962.11	Joback Method
cpg	869.27	J/mol×K	1001.98	Joback Method
cpg	880.19	J/mol×K	1041.85	Joback Method
cpg	889.76	J/mol×K	1081.72	Joback Method
cpg	898.04	J/mol×K	1121.59	Joback Method
cpg	905.08	J/mol×K	1161.46	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=U390084&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