4,4'-Dipropanoyloxydiphenyldiacetylene

Inchi: InChI=1S/C22H18O4/c1-3-21(23)25-19-13-9-17(10-14-19)7-5-6-8-18-11-15-20(16-12-18
InchiKey: YLZSROSRPJTIPP-UHFFFAOYSA-N
Formula: C22H18O4
SMILES: CCC(=O)Oc1ccc(C#CC#Cc2ccc(OC(=O)CC)cc2)cc1
Mol. weight [g/mol]: 346.38
CAS: 92341-24-7

Physical Properties

Property code	Value	Unit	Source
gf	277.68	kJ/mol	Joback Method
hf	7.71	kJ/mol	Joback Method
hfus	51.86	kJ/mol	Joback Method
hvap	93.06	kJ/mol	Joback Method
log10ws	-5.98		Crippen Method
logp	3.721		Crippen Method
mcvol	271.000	ml/mol	McGowan Method
pc	1913.58	kPa	Joback Method
tb	936.66	K	Joback Method
tc	1191.99	K	Joback Method
tf	772.10	K	Joback Method
vc	1.024	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	785.47	J/mol×K	936.66	Joback Method
cpg	798.28	J/mol×K	979.22	Joback Method
cpg	809.59	J/mol×K	1021.77	Joback Method
cpg	819.42	J/mol×K	1064.33	Joback Method
cpg	827.82	J/mol×K	1106.88	Joback Method
cpg	834.83	J/mol×K	1149.44	Joback Method
cpg	840.48	J/mol×K	1191.99	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C92341247&Units=SI
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

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume