4,4'-Dihexanoyloxydiphenyldiacetylene

Inchi: InChI=1S/C28H30O4/c1-3-5-7-13-27(29)31-25-19-15-23(16-20-25)11-9-10-12-24-17-21-
InchiKey: QGHKREKJSWULHP-UHFFFAOYSA-N
Formula: C28H30O4
SMILES: CCCCCC(=O)Oc1ccc(C#CC#Cc2ccc(OC(=O)CCCCC)cc2)cc1
Mol. weight [g/mol]: 430.54
CAS: 92341-26-9

Physical Properties

Property code	Value	Unit	Source
gf	328.20	kJ/mol	Joback Method
hf	-116.13	kJ/mol	Joback Method
hfus	67.40	kJ/mol	Joback Method
hvap	106.41	kJ/mol	Joback Method
log10ws	-8.50		Crippen Method
logp	6.061		Crippen Method
mcvol	355.540	ml/mol	McGowan Method
pc	1220.85	kPa	Joback Method
tb	1073.94	K	Joback Method
tc	1321.16	K	Joback Method
tf	839.72	K	Joback Method
vc	1.359	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1140.12	J/mol×K	1073.94	Joback Method
cpg	1152.59	J/mol×K	1115.14	Joback Method
cpg	1163.46	J/mol×K	1156.35	Joback Method
cpg	1172.79	J/mol×K	1197.55	Joback Method
cpg	1180.66	J/mol×K	1238.76	Joback Method
cpg	1187.12	J/mol×K	1279.96	Joback Method
cpg	1192.25	J/mol×K	1321.16	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=C92341269&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume