4,4'-Dipentanoyloxydiphenyldiacetylene

Inchi: InChI=1S/C26H26O4/c1-3-5-11-25(27)29-23-17-13-21(14-18-23)9-7-8-10-22-15-19-24(2
InchiKey: OVPLFIJMKWNQRE-UHFFFAOYSA-N
Formula: C26H26O4
SMILES: CCCCC(=O)Oc1ccc(C#CC#Cc2ccc(OC(=O)CCCC)cc2)cc1
Mol. weight [g/mol]: 402.48
CAS: 71332-83-7

Physical Properties

Property code	Value	Unit	Source
gf	311.36	kJ/mol	Joback Method
hf	-74.85	kJ/mol	Joback Method
hfus	62.22	kJ/mol	Joback Method
hvap	101.96	kJ/mol	Joback Method
log10ws	-7.66		Crippen Method
logp	5.281		Crippen Method
mcvol	327.360	ml/mol	McGowan Method
pc	1402.74	kPa	Joback Method
tb	1028.18	K	Joback Method
tc	1274.54	K	Joback Method
tf	817.18	K	Joback Method
vc	1.248	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1019.94	J/mol×K	1028.18	Joback Method
cpg	1032.55	J/mol×K	1069.24	Joback Method
cpg	1043.62	J/mol×K	1110.30	Joback Method
cpg	1053.19	J/mol×K	1151.36	Joback Method
cpg	1061.32	J/mol×K	1192.42	Joback Method
cpg	1068.06	J/mol×K	1233.48	Joback Method
cpg	1073.47	J/mol×K	1274.54	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C71332837&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

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