4,4'-Diheptanoyloxydiphenyldiacetylene

Inchi: InChI=1S/C30H34O4/c1-3-5-7-9-15-29(31)33-27-21-17-25(18-22-27)13-11-12-14-26-19-
InchiKey: SUMRTVAVHVZJSN-UHFFFAOYSA-N
Formula: C30H34O4
SMILES: CCCCCCC(=O)Oc1ccc(C#CC#Cc2ccc(OC(=O)CCCCCC)cc2)cc1
Mol. weight [g/mol]: 458.59
CAS: 92341-27-0

Physical Properties

Property code	Value	Unit	Source
gf	345.04	kJ/mol	Joback Method
hf	-157.41	kJ/mol	Joback Method
hfus	72.58	kJ/mol	Joback Method
hvap	110.87	kJ/mol	Joback Method
log10ws	-9.33		Crippen Method
logp	6.841		Crippen Method
mcvol	383.720	ml/mol	McGowan Method
pc	1072.17	kPa	Joback Method
tb	1119.70	K	Joback Method
tc	1371.87	K	Joback Method
tf	862.26	K	Joback Method
vc	1.472	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1261.80	J/mol×K	1119.70	Joback Method
cpg	1274.15	J/mol×K	1161.73	Joback Method
cpg	1284.83	J/mol×K	1203.76	Joback Method
cpg	1293.90	J/mol×K	1245.78	Joback Method
cpg	1301.46	J/mol×K	1287.81	Joback Method
cpg	1307.57	J/mol×K	1329.84	Joback Method
cpg	1312.33	J/mol×K	1371.87	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C92341270&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

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