4,4'-Dibutanoyloxydiphenyldiacetylene

Inchi: InChI=1S/C24H22O4/c1-3-7-23(25)27-21-15-11-19(12-16-21)9-5-6-10-20-13-17-22(18-1
InchiKey: HEEINBGBKKELRM-UHFFFAOYSA-N
Formula: C24H22O4
SMILES: CCCC(=O)Oc1ccc(C#CC#Cc2ccc(OC(=O)CCC)cc2)cc1
Mol. weight [g/mol]: 374.43
CAS: 92341-25-8

Physical Properties

Property code	Value	Unit	Source
gf	294.52	kJ/mol	Joback Method
hf	-33.57	kJ/mol	Joback Method
hfus	57.04	kJ/mol	Joback Method
hvap	97.51	kJ/mol	Joback Method
log10ws	-6.82		Crippen Method
logp	4.501		Crippen Method
mcvol	299.180	ml/mol	McGowan Method
pc	1628.54	kPa	Joback Method
tb	982.42	K	Joback Method
tc	1231.60	K	Joback Method
tf	794.64	K	Joback Method
vc	1.135	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	901.59	J/mol×K	982.42	Joback Method
cpg	914.34	J/mol×K	1023.95	Joback Method
cpg	925.56	J/mol×K	1065.48	Joback Method
cpg	935.32	J/mol×K	1107.01	Joback Method
cpg	943.64	J/mol×K	1148.54	Joback Method
cpg	950.57	J/mol×K	1190.07	Joback Method
cpg	956.17	J/mol×K	1231.60	Joback Method

Sources

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=C92341258&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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