4,4'-Diethanoyloxydiphenyldiacetylene

Inchi: InChI=1S/C20H14O4/c1-15(21)23-19-11-7-17(8-12-19)5-3-4-6-18-9-13-20(14-10-18)24-1
InchiKey: FORJWTANJSWIHA-UHFFFAOYSA-N
Formula: C20H14O4
SMILES: CC(=O)Oc1ccc(C#CC#Cc2ccc(OC(C)=O)cc2)cc1
Mol. weight [g/mol]: 318.32
CAS: 92341-23-6

Physical Properties

Property code	Value	Unit	Source
gf	260.84	kJ/mol	Joback Method
hf	48.99	kJ/mol	Joback Method
hfus	46.68	kJ/mol	Joback Method
hvap	88.61	kJ/mol	Joback Method
log10ws	-5.15		Crippen Method
logp	2.940		Crippen Method
mcvol	242.820	ml/mol	McGowan Method
pc	2280.59	kPa	Joback Method
tb	890.90	K	Joback Method
tc	1155.43	K	Joback Method
tf	749.56	K	Joback Method
vc	0.911	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	672.04	J/mol×K	890.90	Joback Method
cpg	684.77	J/mol×K	934.99	Joback Method
cpg	696.00	J/mol×K	979.08	Joback Method
cpg	705.76	J/mol×K	1023.17	Joback Method
cpg	714.08	J/mol×K	1067.26	Joback Method
cpg	720.99	J/mol×K	1111.34	Joback Method
cpg	726.53	J/mol×K	1155.43	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=C92341236&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