4,4'-Didodecanoyloxydiphenyldiacetylene

Inchi: InChI=1S/C40H54O4/c1-3-5-7-9-11-13-15-17-19-25-39(41)43-37-31-27-35(28-32-37)23-
InchiKey: YYJQUZHMNWZSFS-UHFFFAOYSA-N
Formula: C40H54O4
SMILES: CCCCCCCCCCCC(=O)Oc1ccc(C#CC#Cc2ccc(OC(=O)CCCCCCCCCCC)cc2)cc1
Mol. weight [g/mol]: 598.85
CAS: 92341-29-2

Physical Properties

Property code	Value	Unit	Source
gf	429.24	kJ/mol	Joback Method
hf	-363.81	kJ/mol	Joback Method
hfus	98.48	kJ/mol	Joback Method
hvap	133.13	kJ/mol	Joback Method
log10ws	-13.52		Crippen Method
logp	10.742		Crippen Method
mcvol	524.620	ml/mol	McGowan Method
pc	620.65	kPa	Joback Method
tb	1348.50	K	Joback Method
tc	1707.23	K	Joback Method
tf	401.00 ± 1.00	K	NIST Webbook
vc	2.031	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1884.40	J/mol×K	1348.50	Joback Method
cpg	1897.66	J/mol×K	1408.29	Joback Method
cpg	1908.16	J/mol×K	1468.08	Joback Method
cpg	1916.28	J/mol×K	1527.86	Joback Method
cpg	1922.41	J/mol×K	1587.65	Joback Method
cpg	1926.93	J/mol×K	1647.44	Joback Method
cpg	1930.22	J/mol×K	1707.23	Joback Method
hfust	44.00	kJ/mol	401.00	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C92341292&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
hfust:	Enthalpy of fusion at a given temperature
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