4,4'-Didecanoyloxydiphenyldiacetylene

Inchi: InChI=1S/C36H46O4/c1-3-5-7-9-11-13-15-21-35(37)39-33-27-23-31(24-28-33)19-17-18-
InchiKey: PBQTWTYWXMTXRB-UHFFFAOYSA-N
Formula: C36H46O4
SMILES: CCCCCCCCCC(=O)Oc1ccc(C#CC#Cc2ccc(OC(=O)CCCCCCCCC)cc2)cc1
Mol. weight [g/mol]: 542.75
CAS: 92341-28-1

Physical Properties

Property code	Value	Unit	Source
gf	395.56	kJ/mol	Joback Method
hf	-281.25	kJ/mol	Joback Method
hfus	88.12	kJ/mol	Joback Method
hvap	124.22	kJ/mol	Joback Method
log10ws	-11.84		Crippen Method
logp	9.182		Crippen Method
mcvol	468.260	ml/mol	McGowan Method
pc	758.90	kPa	Joback Method
tb	1256.98	K	Joback Method
tc	1553.80	K	Joback Method
tf	929.88	K	Joback Method
vc	1.808	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1633.18	J/mol×K	1256.98	Joback Method
cpg	1645.67	J/mol×K	1306.45	Joback Method
cpg	1656.00	J/mol×K	1355.92	Joback Method
cpg	1664.33	J/mol×K	1405.39	Joback Method
cpg	1670.84	J/mol×K	1454.86	Joback Method
cpg	1675.72	J/mol×K	1504.33	Joback Method
cpg	1679.14	J/mol×K	1553.80	Joback Method
hfust	42.20	kJ/mol	403.00	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C92341281&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