4,4'-Diundecanoyloxydiphenyldiacetylene

Inchi: InChI=1S/C38H50O4/c1-3-5-7-9-11-13-15-17-23-37(39)41-35-29-25-33(26-30-35)21-19-
InchiKey: BBZPTWIPPJLOMY-UHFFFAOYSA-N
Formula: C38H50O4
SMILES: CCCCCCCCCCC(=O)Oc1ccc(C#CC#Cc2ccc(OC(=O)CCCCCCCCCC)cc2)cc1
Mol. weight [g/mol]: 570.80
CAS: 71332-86-0

Physical Properties

Property code	Value	Unit	Source
gf	412.40	kJ/mol	Joback Method
hf	-322.53	kJ/mol	Joback Method
hfus	93.30	kJ/mol	Joback Method
hvap	128.67	kJ/mol	Joback Method
log10ws	-12.68		Crippen Method
logp	9.962		Crippen Method
mcvol	496.440	ml/mol	McGowan Method
pc	684.57	kPa	Joback Method
tb	1302.74	K	Joback Method
tc	1626.69	K	Joback Method
tf	399.00 ± 1.00	K	NIST Webbook
vc	1.919	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1758.49	J/mol×K	1302.74	Joback Method
cpg	1771.28	J/mol×K	1356.73	Joback Method
cpg	1781.62	J/mol×K	1410.72	Joback Method
cpg	1789.78	J/mol×K	1464.71	Joback Method
cpg	1796.01	J/mol×K	1518.70	Joback Method
cpg	1800.58	J/mol×K	1572.70	Joback Method
cpg	1803.72	J/mol×K	1626.69	Joback Method
hfust	36.20	kJ/mol	399.00	NIST Webbook

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C71332860&Units=SI

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