4,4'-Dinonanoyloxydiphenyldiacetylene

Inchi: InChI=1S/C34H42O4/c1-3-5-7-9-11-13-19-33(35)37-31-25-21-29(22-26-31)17-15-16-18-
InchiKey: ACLSGLFFDMIOJG-UHFFFAOYSA-N
Formula: C34H42O4
SMILES: CCCCCCCCC(=O)Oc1ccc(C#CC#Cc2ccc(OC(=O)CCCCCCCC)cc2)cc1
Mol. weight [g/mol]: 514.69
CAS: 71332-85-9

Physical Properties

Property code	Value	Unit	Source
gf	378.72	kJ/mol	Joback Method
hf	-239.97	kJ/mol	Joback Method
hfus	82.94	kJ/mol	Joback Method
hvap	119.77	kJ/mol	Joback Method
log10ws	-11.01		Crippen Method
logp	8.402		Crippen Method
mcvol	440.080	ml/mol	McGowan Method
pc	846.03	kPa	Joback Method
tb	1211.22	K	Joback Method
tc	1487.55	K	Joback Method
tf	907.34	K	Joback Method
vc	1.696	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1508.53	J/mol×K	1211.22	Joback Method
cpg	1520.88	J/mol×K	1257.28	Joback Method
cpg	1531.26	J/mol×K	1303.33	Joback Method
cpg	1539.82	J/mol×K	1349.39	Joback Method
cpg	1546.68	J/mol×K	1395.44	Joback Method
cpg	1551.97	J/mol×K	1441.50	Joback Method
cpg	1555.83	J/mol×K	1487.55	Joback Method

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=C71332859&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
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