2-(2,4-Hexadiynylidene)-1,6-dioxaspiro[4,4]non-3-

Inchi: InChI=1S/C13H16O2/c1-2-3-4-5-7-12-8-10-13(15-12)9-6-11-14-13/h2-5,7-8,10H,6,9,11H
InchiKey: ZDRLUYUPSIVYOD-ZHMYCGPMSA-N
Formula: C13H16O2
SMILES: CC=CC=CC=C1C=CC2(CCCO2)O1
Mol. weight [g/mol]: 204.26

Physical Properties

Property code	Value	Unit	Source
gf	209.62	kJ/mol	Joback Method
hf	-44.70	kJ/mol	Joback Method
hfus	29.93	kJ/mol	Joback Method
hvap	54.05	kJ/mol	Joback Method
log10ws	-3.74		Crippen Method
logp	3.096		Crippen Method
mcvol	166.850	ml/mol	McGowan Method
pc	2764.26	kPa	Joback Method
rinpol	1875.00		NIST Webbook
tb	596.06	K	Joback Method
tc	833.90	K	Joback Method
tf	343.83	K	Joback Method
vc	0.624	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	423.38	J/mol×K	596.06	Joback Method
cpg	440.37	J/mol×K	635.70	Joback Method
cpg	456.07	J/mol×K	675.34	Joback Method
cpg	470.74	J/mol×K	714.98	Joback Method
cpg	484.63	J/mol×K	754.62	Joback Method
cpg	497.97	J/mol×K	794.26	Joback Method
cpg	511.02	J/mol×K	833.90	Joback Method

Sources

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=R516006&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume