1,6-Dioxaspiro[4,4]nona-2,8-diene, 7-(2,4)-hexadiynylidene

Inchi: InChI=1S/C13H14O2/c1-2-3-4-5-7-12-8-10-13(15-12)9-6-11-14-13/h2-8,10-11H,9H2,1H3

InchiKey: MDHFLFFAHKTMIR-UAJIGUHOSA-N

Formula: C13H14O2

SMILES: CC=CC=CC=C1C=CC2(CC=CO2)O1

Mol. weight [g/mol]: 202.25

Physical Properties

Property code	Value	Unit	Source
gf	239.58	kJ/mol	Joback Method
hf	13.08	kJ/mol	Joback Method
hfus	31.16	kJ/mol	Joback Method
hvap	54.34	kJ/mol	Joback Method
log10ws	-4.09		Crippen Method
logp	3.219		Crippen Method
mcvol	162.550	ml/mol	McGowan Method
pc	2871.95	kPa	Joback Method
rinpol	1789.00		NIST Webbook
rinpol	1799.00		NIST Webbook
rinpol	1789.00		NIST Webbook
tb	595.22	K	Joback Method
tc	835.42	K	Joback Method
tf	344.59	K	Joback Method
vc	0.610	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	402.85	J/mol×K	595.22	Joback Method
cpg	418.60	J/mol×K	635.25	Joback Method
cpg	433.11	J/mol×K	675.29	Joback Method
cpg	446.63	J/mol×K	715.32	Joback Method
cpg	459.43	J/mol×K	755.36	Joback Method
cpg	471.75	J/mol×K	795.39	Joback Method
cpg	483.85	J/mol×K	835.42	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=R199849&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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