(Z)-2-(Hexa-2,4-diyn-1-ylidene)-1,6-dioxaspiro[4.4]

Other names: cis-ene-yne-Dicycloether
(Z)-ene-yne-Dicycloether
(Z)-Tonghaosu
Inchi: InChI=1S/C13H12O2/c1-2-3-4-5-7-12-8-10-13(15-12)9-6-11-14-13/h7-8,10H,6,9,11H2,1
InchiKey: WTRXKCNFPMTAJV-GHXNOFRVSA-N
Formula: C13H12O2
SMILES: CC#CC#CC=C1C=CC2(CCCO2)O1
Mol. weight [g/mol]: 200.23
CAS: 4575-53-5

Physical Properties

Property code	Value	Unit	Source
gf	454.78	kJ/mol	Joback Method
hf	265.46	kJ/mol	Joback Method
hfus	35.77	kJ/mol	Joback Method
hvap	58.44	kJ/mol	Joback Method
log10ws	-3.63		Crippen Method
logp	1.990		Crippen Method
mcvol	158.250	ml/mol	McGowan Method
pc	3517.91	kPa	Joback Method
rinpol	1807.00		NIST Webbook
rinpol	1891.20		NIST Webbook
rinpol	1891.20		NIST Webbook
tb	605.74	K	Joback Method
tc	884.24	K	Joback Method
tf	566.19	K	Joback Method
vc	0.588	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	384.13	J/mol×K	605.74	Joback Method
cpg	400.74	J/mol×K	652.16	Joback Method
cpg	416.09	J/mol×K	698.57	Joback Method

cpg	430.51	J/mol×K	744.99	Joback Method
cpg	444.31	J/mol×K	791.41	Joback Method
cpg	457.79	J/mol×K	837.83	Joback Method
cpg	471.28	J/mol×K	884.24	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=C4575535&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