cis-En-yn-dicycloether

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

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	1846.00		NIST Webbook
rinpol	1843.00		NIST Webbook
rinpol	1802.00		NIST Webbook
rinpol	1808.00		NIST Webbook
rinpol	1808.00		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: 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=R203171&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