Spiro-ether

Inchi: InChI=1S/C13H14O2/c1-2-3-4-5-7-12-8-10-13(15-12)9-6-11-14-13/h8,10,12H,6-7,9,11H2
InchiKey: NJLYCNZOTQCQMC-UHFFFAOYSA-N
Formula: C13H14O2
SMILES: CC#CC#CCC1C=CC2(CCCO2)O1
Mol. weight [g/mol]: 202.25

Physical Properties

Property code	Value	Unit	Source
gf	401.61	kJ/mol	Joback Method
hf	169.09	kJ/mol	Joback Method
hfus	36.52	kJ/mol	Joback Method
hvap	57.34	kJ/mol	Joback Method
log10ws	-3.39		Crippen Method
logp	1.865		Crippen Method
mcvol	162.550	ml/mol	McGowan Method
pc	3272.78	kPa	Joback Method
rinpol	1805.00		NIST Webbook
rinpol	1804.00		NIST Webbook
rinpol	1805.00		NIST Webbook
rinpol	1804.00		NIST Webbook
tb	594.43	K	Joback Method
tc	864.18	K	Joback Method
tf	551.59	K	Joback Method
vc	0.604	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	407.35	J/mol×K	594.43	Joback Method
cpg	425.92	J/mol×K	639.39	Joback Method
cpg	443.11	J/mol×K	684.35	Joback Method
cpg	459.18	J/mol×K	729.31	Joback Method
cpg	474.41	J/mol×K	774.26	Joback Method
cpg	489.07	J/mol×K	819.22	Joback Method

cpg	503.41	J/mol×K	864.18	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=R600567&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