(E)-Tibetin spiroether

Inchi: InChI=1S/C14H14O2/c1-2-3-4-5-6-8-13-9-11-14(16-13)10-7-12-15-14/h8-9,11H,2,7,10,1
InchiKey: SDEBTHGVRKGQTB-MDWZMJQESA-N
Formula: C14H14O2
SMILES: CCC#CC#CC=C1C=CC2(CCCO2)O1
Mol. weight [g/mol]: 214.26

Physical Properties

Property code	Value	Unit	Source
gf	463.20	kJ/mol	Joback Method
hf	244.82	kJ/mol	Joback Method
hfus	38.36	kJ/mol	Joback Method
hvap	60.66	kJ/mol	Joback Method
log10ws	-4.05		Crippen Method
logp	2.380		Crippen Method
mcvol	172.340	ml/mol	McGowan Method
pc	3149.09	kPa	Joback Method
rinpol	1888.00		NIST Webbook
tb	628.62	K	Joback Method
tc	900.08	K	Joback Method
tf	577.46	K	Joback Method
vc	0.643	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	432.76	J/mol×K	628.62	Joback Method
cpg	450.10	J/mol×K	673.86	Joback Method
cpg	466.27	J/mol×K	719.11	Joback Method
cpg	481.56	J/mol×K	764.35	Joback Method
cpg	496.27	J/mol×K	809.60	Joback Method
cpg	510.70	J/mol×K	854.84	Joback Method
cpg	525.15	J/mol×K	900.08	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R270052&Units=SI
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

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