

# (Z)-Tibetin spiroether

<b>Inchi:</b>	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
<b>InchiKey:</b>	SDEBTHGVRKQGQB-JYRVWZFOA-N
<b>Formula:</b>	C14H14O2
<b>SMILES:</b>	CCC#CC#CC=C1C=CC2(CCCO2)O1
<b>Mol. weight [g/mol]:</b>	214.26
<b>CAS:</b>	206062-16-0

## 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	1836.00		NIST Webbook
rinpol	1925.60		NIST Webbook
rinpol	1925.60		NIST Webbook
rinpol	1836.00		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/molxK	628.62	Joback Method
cpg	450.10	J/molxK	673.86	Joback Method
cpg	466.27	J/molxK	719.11	Joback Method
cpg	481.56	J/molxK	764.35	Joback Method
cpg	496.27	J/molxK	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

<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C206062160&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C206062160&amp;Units=SI</a>

## Legend

<b>cpg:</b>	Ideal gas heat capacity
<b>gf:</b>	Standard Gibbs free energy of formation
<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hfus:</b>	Enthalpy of fusion at standard conditions
<b>hvac:</b>	Enthalpy of vaporization at standard conditions
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>rinpol:</b>	Non-polar retention indices
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

Latest version available from:

<https://www.chemeo.com/cid/82-518-6/Z-Tibetin-spiroether.pdf>

Generated by Cheméo on 2024-04-19 22:23:41.648543415 +0000 UTC m=+15854670.569120729.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.