

# (E)-Theaspirane

<b>Other names:</b>	trans-theaspirane
<b>Inchi:</b>	InChI=1S/C13H22O/c1-10-6-5-8-12(3,4)13(10)9-7-11(2)14-13/h6,11H,5,7-9H2,1-4H3/t1
<b>InchiKey:</b>	GYUZHTWCNKINPY-YPMHNCESA-N
<b>Formula:</b>	C13H22O
<b>SMILES:</b>	CC1=CCCC(C)(C)C12CCC(C)O2
<b>Mol. weight [g/mol]:</b>	194.31

## Physical Properties

Property code	Value	Unit	Source
gf	47.20	kJ/mol	Joback Method
hf	-266.24	kJ/mol	Joback Method
hfus	14.58	kJ/mol	Joback Method
hvap	47.90	kJ/mol	Joback Method
log10ws	-3.98		Crippen Method
logp	3.690		Crippen Method
mcvol	173.880	ml/mol	McGowan Method
pc	2410.00	kPa	Joback Method
ripol	1375.00		NIST Webbook
ripol	1303.00		NIST Webbook
ripol	1375.00		NIST Webbook
ripol	1498.00		NIST Webbook
ripol	1491.00		NIST Webbook
ripol	1516.00		NIST Webbook
ripol	1491.00		NIST Webbook
ripol	1543.00		NIST Webbook
ripol	1516.00		NIST Webbook
ripol	1543.00		NIST Webbook
ripol	1498.00		NIST Webbook
ripol	1516.00		NIST Webbook
ripol	1516.00		NIST Webbook
tb	554.30	K	Joback Method
tc	785.37	K	Joback Method
tf	341.48	K	Joback Method
vc	0.647	m <sup>3</sup> /kmol	Joback Method

# Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	451.24	J/mol×K	554.30	Joback Method
cpg	473.01	J/mol×K	592.81	Joback Method
cpg	493.29	J/mol×K	631.32	Joback Method
cpg	512.34	J/mol×K	669.83	Joback Method
cpg	530.43	J/mol×K	708.35	Joback Method
cpg	547.81	J/mol×K	746.86	Joback Method
cpg	564.75	J/mol×K	785.37	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=R54862&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R54862&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>hvap:</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>ripol:</b>	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

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