

# Atis-16-ene, (5«beta»,8«alpha»,9«beta»,10«alpha»,12«alpha»)-

Other names:

5«beta»,9«beta»,10«alpha»-Atis-16-ene

(-)-Atisirene

Atiserene

5«beta»,8«alpha»,9«beta»,10«alpha»,12«alpha»-Atis-16-ene

Inchi: InChI=1S/C20H32/c1-14-13-20-10-6-15(14)12-17(20)19(4)9-5-8-18(2,3)16(19)7-11-20/h

InchiKey: LFRRLVVLXYROS-UHFFFAOYSA-N

Formula: C20H32

SMILES: C=C1CC23CCC1CC2C1(C)CCCC(C)(C)C1CC3

Mol. weight [g/mol]: 272.47

CAS: 20230-48-2

## Physical Properties

Property code	Value	Unit	Source
gf	333.31	kJ/mol	Joback Method
hf	-100.29	kJ/mol	Joback Method
hfus	13.79	kJ/mol	Joback Method
hvap	56.54	kJ/mol	Joback Method
log10ws	-6.18		Crippen Method
logp	5.975		Crippen Method
mcvol	244.920	ml/mol	McGowan Method
pc	1693.51	kPa	Joback Method
rinpol	2010.00		NIST Webbook
tb	691.58	K	Joback Method
tc	933.36	K	Joback Method
tf	449.74	K	Joback Method
vc	0.927	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	768.47	J/molxK	691.58	Joback Method
cpg	795.89	J/molxK	731.88	Joback Method
cpg	822.42	J/molxK	772.17	Joback Method
cpg	848.59	J/molxK	812.47	Joback Method

cpg	874.91	J/mol×K	852.76	Joback Method
cpg	901.90	J/mol×K	893.06	Joback Method
cpg	930.06	J/mol×K	933.36	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=C20230482&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C20230482&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>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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