

# 4,6,8-Trimethylazulene

<b>Other names:</b>	Azulene, 4,6,8-trimethyl- 2,4,6-Trimethylbicyclo(5.3.0)deca-2,4,6,8,10-pentaene
<b>Inchi:</b>	InChI=1S/C13H14/c1-9-7-10(2)12-5-4-6-13(12)11(3)8-9/h4-8H,1-3H3
<b>InchiKey:</b>	RUNBRXWUHPOTOO-UHFFFAOYSA-N
<b>Formula:</b>	C13H14
<b>SMILES:</b>	<chem>Cc1cc(C)c2cccc-2c(C)c1</chem>
<b>Mol. weight [g/mol]:</b>	170.25
<b>CAS:</b>	941-81-1

## Physical Properties

Property code	Value	Unit	Source
gf	248.75	kJ/mol	Joback Method
hf	81.54	kJ/mol	Joback Method
hfus	19.32	kJ/mol	Joback Method
hvap	50.43	kJ/mol	Joback Method
ie	7.10	eV	NIST Webbook
log10ws	-4.92		Crippen Method
logp	3.717		Crippen Method
mcvol	150.810	ml/mol	McGowan Method
pc	2670.78	kPa	Joback Method
rinpol	1659.00		NIST Webbook
rinpol	1638.00		NIST Webbook
tb	557.44	K	Joback Method
tc	785.77	K	Joback Method
tf	332.95	K	Joback Method
vc	0.578	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	342.00	J/molxK	557.44	Joback Method
cpg	357.34	J/molxK	595.49	Joback Method
cpg	371.70	J/molxK	633.55	Joback Method
cpg	385.15	J/molxK	671.60	Joback Method

cpg	397.73	J/molxK	709.66	Joback Method
cpg	409.52	J/molxK	747.71	Joback Method
cpg	420.56	J/molxK	785.77	Joback Method
dvisc	0.0010939	Paxs	332.95	Joback Method
dvisc	0.0007795	Paxs	370.37	Joback Method
dvisc	0.0005911	Paxs	407.78	Joback Method
dvisc	0.0004696	Paxs	445.20	Joback Method
dvisc	0.0003866	Paxs	482.61	Joback Method
dvisc	0.0003273	Paxs	520.03	Joback Method
dvisc	0.0002834	Paxs	557.44	Joback Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C941811&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C941811&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</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>

## Legend

<b>cpg:</b>	Ideal gas heat capacity
<b>dvisc:</b>	Dynamic viscosity
<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>ie:</b>	Ionization energy
<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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