

## [3.3.3]Propellane, 2,8,9-tris(methylene)-

<b>Inchi:</b>	InChI=1S/C14H18/c1-10-4-7-13-8-5-11(2)14(10,13)12(3)6-9-13/h1-9H2
<b>InchiKey:</b>	QZCISUCJHQWIHV-UHFFFAOYSA-N
<b>Formula:</b>	C14H18
<b>SMILES:</b>	C=C1CCC23CCC(=C)C12C(=C)CC3
<b>Mol. weight [g/mol]:</b>	186.29
<b>CAS:</b>	58461-87-3

## Physical Properties

Property code	Value	Unit	Source
gf	381.02	kJ/mol	Joback Method
hf	177.33	kJ/mol	Joback Method
hfus	5.08	kJ/mol	Joback Method
hvap	45.33	kJ/mol	Joback Method
ie	8.40	eV	NIST Webbook
ie	8.90	eV	NIST Webbook
log10ws	-4.44		Crippen Method
logp	4.009		Crippen Method
mcvol	162.640	ml/mol	McGowan Method
pc	2651.56	kPa	Joback Method
tb	551.11	K	Joback Method
tc	783.90	K	Joback Method
tf	387.40	K	Joback Method
vc	0.624	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	409.23	J/molxK	551.11	Joback Method
cpg	427.92	J/molxK	589.91	Joback Method
cpg	445.11	J/molxK	628.71	Joback Method
cpg	461.11	J/molxK	667.51	Joback Method
cpg	476.24	J/molxK	706.30	Joback Method
cpg	490.84	J/molxK	745.10	Joback Method
cpg	505.24	J/molxK	783.90	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=C58461873&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C58461873&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>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>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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