

# Pethybrene

Inchi:

InChI=1S/C15H24/c1-11-6-9-13(3)10-12(2)14(4)7-5-8-15(11,13)14/h11H,2,5-10H2,1,3-4H

InchiKey:

BPSJFUIWVOWJNO-ZGKBOVNRSA-N

Formula:

C15H24

SMILES:

C=C1CC2(C)CCC(C)C23CCCC13C

Mol. weight [g/mol]:

204.35

## Physical Properties

Property code	Value	Unit	Source
gf	262.37	kJ/mol	Joback Method
hf	-37.23	kJ/mol	Joback Method
hfus	5.83	kJ/mol	Joback Method
hvap	45.46	kJ/mol	Joback Method
log10ws	-4.67		Crippen Method
logp	4.559		Crippen Method
mcvol	185.330	ml/mol	McGowan Method
pc	2274.07	kPa	Joback Method
rinpol	1377.00		NIST Webbook
rinpol	1377.00		NIST Webbook
rinpol	1362.00		NIST Webbook
rinpol	1371.00		NIST Webbook
rinpol	1377.00		NIST Webbook
ripol	1512.00		NIST Webbook
ripol	1512.00		NIST Webbook
tb	566.57	K	Joback Method
tc	800.20	K	Joback Method
tf	386.73	K	Joback Method
vc	0.708	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	500.14	J/molxK	566.57	Joback Method
cpg	522.76	J/molxK	605.51	Joback Method
cpg	543.69	J/molxK	644.45	Joback Method

cpg	563.39	J/mol×K	683.38	Joback Method
cpg	582.28	J/mol×K	722.32	Joback Method
cpg	600.82	J/mol×K	761.26	Joback Method
cpg	619.44	J/mol×K	800.20	Joback Method

## Sources

<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=R417157&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R417157&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>

## 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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