

# Pyrene, hexadecahydro-

<b>Other names:</b>	Hexadecahydropyrene Perhydropyrene
<b>Inchi:</b>	InChI=1S/C16H26/c1-3-11-7-9-13-5-2-6-14-10-8-12(4-1)15(11)16(13)14/h11-16H,1-10H2
<b>InchiKey:</b>	BYBPEZLZCGOWIS-UHFFFAOYSA-N
<b>Formula:</b>	C16H26
<b>SMILES:</b>	C1CC2CCC3CCCC4CCC(C1)C2C34
<b>Mol. weight [g/mol]:</b>	218.38
<b>CAS:</b>	2435-85-0

## Physical Properties

Property code	Value	Unit	Source
gf	263.02	kJ/mol	Joback Method
hf	-147.69	kJ/mol	Joback Method
hfus	23.48	kJ/mol	Joback Method
hvap	50.93	kJ/mol	Joback Method
log10ws	-4.65		Crippen Method
logp	4.639		Crippen Method
mvol	192.860	ml/mol	McGowan Method
pc	2066.12	kPa	Joback Method
tb	600.18	K	Joback Method
tc	832.27	K	Joback Method
tf	319.28	K	Joback Method
vc	0.726	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	571.83	J/mol×K	600.18	Joback Method
cpg	599.84	J/mol×K	638.86	Joback Method
cpg	625.86	J/mol×K	677.54	Joback Method
cpg	650.04	J/mol×K	716.22	Joback Method
cpg	672.51	J/mol×K	754.90	Joback Method
cpg	693.41	J/mol×K	793.58	Joback Method
cpg	712.88	J/mol×K	832.27	Joback Method

dvisc	0.0026326	Paxs	319.28	Joback Method
dvisc	0.0025174	Paxs	366.10	Joback Method
dvisc	0.0024318	Paxs	412.91	Joback Method
dvisc	0.0023657	Paxs	459.73	Joback Method
dvisc	0.0023131	Paxs	506.55	Joback Method
dvisc	0.0022704	Paxs	553.36	Joback Method
dvisc	0.0022349	Paxs	600.18	Joback Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C2435850&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C2435850&amp;Units=SI</a>
<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>

## 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>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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