

# 3H-Benzo[cd]pyrene

<b>Inchi:</b>	InChI=1S/C19H12/c1-3-12-7-9-14-10-8-13-4-2-6-16-11-15(5-1)17(12)19(14)18(13)16/h1
<b>InchiKey:</b>	LFBJZFWBDRYIY-UHFFFAOYSA-N
<b>Formula:</b>	C19H12
<b>SMILES:</b>	<chem>C1=Cc2cc3cccc4ccc5ccc(c2c5c43)C1</chem>
<b>Mol. weight [g/mol]:</b>	240.30
<b>CAS:</b>	191-35-5

## Physical Properties

Property code	Value	Unit	Source
gf	595.60	kJ/mol	Joback Method
hf	433.83	kJ/mol	Joback Method
hfus	29.77	kJ/mol	Joback Method
hvap	67.61	kJ/mol	Joback Method
log10ws	-7.40		Crippen Method
logp	5.153		Crippen Method
mvol	185.570	ml/mol	McGowan Method
pc	2704.22	kPa	Joback Method
tb	740.53	K	Joback Method
tc	999.94	K	Joback Method
tf	507.71	K	Joback Method
vc	0.732	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	492.08	J/molxK	740.53	Joback Method
cpg	505.43	J/molxK	783.76	Joback Method
cpg	517.99	J/molxK	827.00	Joback Method
cpg	530.06	J/molxK	870.23	Joback Method
cpg	541.90	J/molxK	913.47	Joback Method
cpg	553.80	J/molxK	956.70	Joback Method
cpg	566.02	J/molxK	999.94	Joback Method
dvisc	0.0038035	Paxs	507.71	Joback Method
dvisc	0.0036267	Paxs	546.51	Joback Method

dvisc	0.0034800	Paxs	585.32	Joback Method
dvisc	0.0033565	Paxs	624.12	Joback Method
dvisc	0.0032511	Paxs	662.92	Joback Method
dvisc	0.0031601	Paxs	701.73	Joback Method
dvisc	0.0030808	Paxs	740.53	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=C191355&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C191355&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>

## 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>mccvol:</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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