

# 1H-Benzo[ghi]cyclopenta[pqr]perylene

<b>Inchi:</b>	InChI=1S/C23H12/c1-2-13-4-6-15-8-10-17-11-16-9-7-14-5-3-12(1)18-19(13)21(15)23(17)
<b>InchiKey:</b>	VLWBVWWYQNHWKN-UHFFFAOYSA-N
<b>Formula:</b>	C23H12
<b>SMILES:</b>	c1cc2ccc3ccc4ccc5ccc6c7c(c1C6)c2c3c4c57
<b>Mol. weight [g/mol]:</b>	288.34
<b>CAS:</b>	64503-02-2

## Physical Properties

Property code	Value	Unit	Source
gf	811.80	kJ/mol	Joback Method
hf	619.55	kJ/mol	Joback Method
hfus	39.35	kJ/mol	Joback Method
hvap	79.85	kJ/mol	Joback Method
log10ws	-9.67		Crippen Method
logp	6.232		Crippen Method
mcvol	211.610	ml/mol	McGowan Method
pc	2453.17	kPa	Joback Method
tb	864.57	K	Joback Method
tc	1124.44	K	Joback Method
tf	655.79	K	Joback Method
vc	0.860	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	595.47	J/molxK	864.57	Joback Method
cpg	673.43	J/molxK	1081.13	Joback Method
cpg	654.88	J/molxK	1037.82	Joback Method
cpg	638.22	J/molxK	994.51	Joback Method
cpg	623.04	J/molxK	951.19	Joback Method
cpg	608.93	J/molxK	907.88	Joback Method
cpg	694.28	J/molxK	1124.44	Joback Method
dvisc	0.0426312	Paxs	864.57	Joback Method
dvisc	0.0413228	Paxs	829.77	Joback Method

dvisc	0.0399454	Paxs	794.98	Joback Method
dvisc	0.0384942	Paxs	760.18	Joback Method
dvisc	0.0369643	Paxs	725.38	Joback Method
dvisc	0.0353505	Paxs	690.59	Joback Method
dvisc	0.0336473	Paxs	655.79	Joback Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C64503022&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C64503022&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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