

# Tetrabenzo[a,f,j,o]perylene

<b>Inchi:</b>	InChI=1S/C36H20/c1-5-13-27-21(9-1)17-25-18-22-10-2-7-15-29(22)35-31(25)33(27)34-2
<b>InchiKey:</b>	MWLMHSGPMCQCFJ-UHFFFAOYSA-N
<b>Formula:</b>	C36H20
<b>SMILES:</b>	c1ccc2c(c1)cc1cc3ccccc3c3c1c2c1c2ccccc2cc2cc4ccccc4c3c21
<b>Mol. weight [g/mol]:</b>	452.54
<b>CAS:</b>	191-03-7

## Physical Properties

Property code	Value	Unit	Source
gf	1144.68	kJ/mol	Joback Method
hf	852.97	kJ/mol	Joback Method
hfus	59.44	kJ/mol	Joback Method
hvap	115.12	kJ/mol	Joback Method
log10ws	-15.32		Crippen Method
logp	10.350		Crippen Method
mvol	342.960	ml/mol	McGowan Method
pc	1509.33	kPa	Joback Method
tb	1228.76	K	Joback Method
tc	1519.31	K	Joback Method
tf	877.42	K	Joback Method
vc	1.349	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1176.13	J/molxK	1228.76	Joback Method
cpg	1425.02	J/molxK	1470.89	Joback Method
cpg	1362.92	J/molxK	1422.46	Joback Method
cpg	1307.64	J/molxK	1374.04	Joback Method
cpg	1258.52	J/molxK	1325.61	Joback Method
cpg	1214.90	J/molxK	1277.19	Joback Method
cpg	1494.62	J/molxK	1519.31	Joback Method
dvisc	0.0184030	Paxs	1228.76	Joback Method
dvisc	0.0189069	Paxs	1170.20	Joback Method

dvisc	0.0194799	Paxs	1111.65	Joback Method
dvisc	0.0201371	Paxs	1053.09	Joback Method
dvisc	0.0208980	Paxs	994.53	Joback Method
dvisc	0.0217885	Paxs	935.98	Joback Method
dvisc	0.0228438	Paxs	877.42	Joback Method

## Sources

<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=C191037&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C191037&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>

## 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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