

# Tribenzo[b,n,pqr]perylene

<b>Inchi:</b>	InChI=1S/C30H16/c1-3-9-19-17(7-1)21-11-5-13-23-24-14-6-12-22-18-8-2-4-10-20(18)26
<b>InchiKey:</b>	OCHHCTQLQKUZZD-UHFFFAOYSA-N
<b>Formula:</b>	C30H16
<b>SMILES:</b>	c1ccc2c(c1)c1cccc3c4cccc5c6cccc6c6ccc2c(c13)c6c54
<b>Mol. weight [g/mol]:</b>	376.45
<b>CAS:</b>	190-81-8

## Physical Properties

Property code	Value	Unit	Source
gf	991.38	kJ/mol	Joback Method
hf	751.75	kJ/mol	Joback Method
hfus	50.25	kJ/mol	Joback Method
hvap	98.83	kJ/mol	Joback Method
ie	7.13	eV	NIST Webbook
ie	7.13	eV	NIST Webbook
ie	7.13	eV	NIST Webbook
log10ws	-12.93		Crippen Method
logp	8.635		Crippen Method
mcvol	282.180	ml/mol	McGowan Method
pc	1867.55	kPa	Joback Method
tb	1059.82	K	Joback Method
tc	1334.83	K	Joback Method
tf	770.86	K	Joback Method
vc	1.121	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	877.53	J/molxK	1059.82	Joback Method
cpg	900.56	J/molxK	1105.65	Joback Method
cpg	926.04	J/molxK	1151.49	Joback Method
cpg	954.48	J/molxK	1197.32	Joback Method
cpg	986.42	J/molxK	1243.16	Joback Method
cpg	1022.37	J/molxK	1288.99	Joback Method

cpg	1062.84	J/mol×K	1334.83	Joback Method
dvisc	0.0277526	Paxs	770.86	Joback Method
dvisc	0.0275076	Paxs	819.02	Joback Method
dvisc	0.0272917	Paxs	867.18	Joback Method
dvisc	0.0270999	Paxs	915.34	Joback Method
dvisc	0.0269285	Paxs	963.50	Joback Method
dvisc	0.0267743	Paxs	1011.66	Joback Method
dvisc	0.0266349	Paxs	1059.82	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=C190818&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C190818&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>ie:</b>	Ionization energy
<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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