

# Anthra[3,2,1,9-pqra]benzo[cd]perylene

<b>Inchi:</b>	InChI=1S/C32H16/c1-2-8-22-19(5-1)15-21-16-20-12-11-17-6-3-9-23-24-14-13-18-7-4-10
<b>InchiKey:</b>	MTSCSWCMANISGO-UHFFFAOYSA-N
<b>Formula:</b>	C32H16
<b>SMILES:</b>	c1ccc2c(c1)cc1cc3ccc4cccc5c6ccc7cccc8c7c6c(c3c45)c1c28
<b>Mol. weight [g/mol]:</b>	400.47
<b>CAS:</b>	120836-18-2

## Physical Properties

Property code	Value	Unit	Source
gf	1099.48	kJ/mol	Joback Method
hf	844.61	kJ/mol	Joback Method
hfus	55.04	kJ/mol	Joback Method
hvap	104.95	kJ/mol	Joback Method
log10ws	-14.15		Crippen Method
logp	9.226		Crippen Method
mvol	295.200	ml/mol	McGowan Method
pc	1792.42	kPa	Joback Method
tb	1121.84	K	Joback Method
tc	1399.15	K	Joback Method
tf	844.90	K	Joback Method
vc	1.185	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	953.39	J/molxK	1121.84	Joback Method
cpg	984.02	J/molxK	1168.06	Joback Method
cpg	1018.68	J/molxK	1214.28	Joback Method
cpg	1057.97	J/molxK	1260.50	Joback Method
cpg	1102.53	J/molxK	1306.71	Joback Method
cpg	1152.95	J/molxK	1352.93	Joback Method
cpg	1209.85	J/molxK	1399.15	Joback Method
dvisc	0.1009143	Paxs	844.90	Joback Method
dvisc	0.1032630	Paxs	891.06	Joback Method

dvisc	0.1054271	Paxs	937.21	Joback Method
dvisc	0.1074272	Paxs	983.37	Joback Method
dvisc	0.1092809	Paxs	1029.53	Joback Method
dvisc	0.1110035	Paxs	1075.68	Joback Method
dvisc	0.1126083	Paxs	1121.84	Joback Method

## Sources

<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>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C120836182&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C120836182&amp;Units=SI</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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