

# Tribenzo[a,ef,hi]coronene

<b>Inchi:</b>	InChI=1S/C34H16/c1-2-8-22-21(7-1)25-14-13-17-11-12-20-15-18-5-3-9-23-24-10-4-6-19
<b>InchiKey:</b>	UGIIKSPAEBLJKF-UHFFFAOYSA-N
<b>Formula:</b>	C34H16
<b>SMILES:</b>	<chem>c1ccc2c(c1)c1ccc3ccc4cc5cccc6c7cccc8cc2c2c1c3c4c(c56)c2c87</chem>
<b>Mol. weight [g/mol]:</b>	424.49
<b>CAS:</b>	128345-70-0

## Physical Properties

Property code	Value	Unit	Source
gf	1207.58	kJ/mol	Joback Method
hf	937.47	kJ/mol	Joback Method
hfus	59.83	kJ/mol	Joback Method
hvap	111.07	kJ/mol	Joback Method
log10ws	-15.37		Crippen Method
logp	9.817		Crippen Method
mvol	308.220	ml/mol	McGowan Method
pc	1721.73	kPa	Joback Method
tb	1183.86	K	Joback Method
tc	1465.19	K	Joback Method
tf	918.94	K	Joback Method
vc	1.250	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1044.98	J/molxK	1183.86	Joback Method
cpg	1086.84	J/molxK	1230.75	Joback Method
cpg	1134.65	J/molxK	1277.64	Joback Method
cpg	1189.14	J/molxK	1324.53	Joback Method
cpg	1251.03	J/molxK	1371.42	Joback Method
cpg	1321.06	J/molxK	1418.30	Joback Method
cpg	1399.93	J/molxK	1465.19	Joback Method
dvisc	0.4024121	Paxs	918.94	Joback Method
dvisc	0.4201945	Paxs	963.09	Joback Method

dvisc	0.4371025	Paxs	1007.25	Joback Method
dvisc	0.4531868	Paxs	1051.40	Joback Method
dvisc	0.4684964	Paxs	1095.55	Joback Method
dvisc	0.4830780	Paxs	1139.71	Joback Method
dvisc	0.4969759	Paxs	1183.86	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.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.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=C128345700&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C128345700&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>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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