

# Anthra[2,1-a]aceanthrylene

<b>Inchi:</b>	InChI=1S/C28H16/c1-2-7-18-16-25-20(14-17(18)6-1)12-13-24-27(25)23-11-5-9-21-15-19
<b>InchiKey:</b>	VPHATVBTDPUCM-UHFFFAOYSA-N
<b>Formula:</b>	C28H16
<b>SMILES:</b>	<chem>c1ccc2cc3c4c(ccc3cc2c1)-c1c2ccccc2cc2cccc-4c12</chem>
<b>Mol. weight [g/mol]:</b>	352.43
<b>CAS:</b>	203-21-4

## Physical Properties

Property code	Value	Unit	Source
gf	883.28	kJ/mol	Joback Method
hf	658.89	kJ/mol	Joback Method
hfus	45.46	kJ/mol	Joback Method
hvap	92.71	kJ/mol	Joback Method
log10ws	-12.14		Crippen Method
logp	7.947		Crippen Method
mcvol	269.160	ml/mol	McGowan Method
pc	1947.51	kPa	Joback Method
tb	997.80	K	Joback Method
tc	1271.87	K	Joback Method
tf	696.82	K	Joback Method
vc	1.058	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	812.33	J/molxK	997.80	Joback Method
cpg	919.98	J/molxK	1226.19	Joback Method
cpg	894.41	J/molxK	1180.51	Joback Method
cpg	871.30	J/molxK	1134.83	Joback Method
cpg	850.20	J/molxK	1089.16	Joback Method
cpg	830.69	J/molxK	1043.48	Joback Method
cpg	948.44	J/molxK	1271.87	Joback Method
dvisc	0.0066304	Paxs	997.80	Joback Method
dvisc	0.0068476	Paxs	947.64	Joback Method

dvisc	0.0070975	Paxs	897.47	Joback Method
dvisc	0.0073878	Paxs	847.31	Joback Method
dvisc	0.0077289	Paxs	797.15	Joback Method
dvisc	0.0081349	Paxs	746.98	Joback Method
dvisc	0.0086256	Paxs	696.82	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=C203214&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C203214&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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