

# Chrysene, 5-methyl-

<b>Other names:</b>	5-Methylchrysene
<b>Inchi:</b>	InChI=1S/C19H14/c1-13-12-15-7-3-4-8-16(15)18-11-10-14-6-2-5-9-17(14)19(13)18/h2-12
<b>InchiKey:</b>	GOHBXWHNJHENRX-UHFFFAOYSA-N
<b>Formula:</b>	C19H14
<b>SMILES:</b>	<chem>Cc1cc2ccccc2c2ccc3ccccc3c12</chem>
<b>Mol. weight [g/mol]:</b>	242.31
<b>CAS:</b>	3697-24-3

## Physical Properties

Property code	Value	Unit	Source
gf	512.57	kJ/mol	Joback Method
hf	339.84	kJ/mol	Joback Method
hfus	28.90	kJ/mol	Joback Method
hvap	67.07	kJ/mol	Joback Method
ie	7.40 ± 0.03	eV	NIST Webbook
log10ws	-6.59		Aqueous Solubility Prediction Method
log10ws	-6.59		Estimated Solubility Method
logp	5.455		Crippen Method
mcvol	196.430	ml/mol	McGowan Method
pc	2448.32	kPa	Joback Method
rinpola	418.67		NIST Webbook
rinpola	418.67		NIST Webbook
rinpola	420.01		NIST Webbook
rinpola	419.00		NIST Webbook
rinpola	419.68		NIST Webbook
rinpola	420.20		NIST Webbook
rinpola	420.40		NIST Webbook
rinpola	419.68		NIST Webbook
rinpola	419.00		NIST Webbook
tb	732.68	K	Joback Method
tc	990.82	K	Joback Method
tf	391.00 ± 1.00	K	NIST Webbook
tf	389.00 ± 4.00	K	NIST Webbook
vc	0.757	m <sup>3</sup> /kmol	Joback Method

# Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	597.11	J/molxK	990.82	Joback Method
cpg	585.49	J/molxK	947.80	Joback Method
cpg	573.55	J/molxK	904.77	Joback Method
cpg	561.09	J/molxK	861.75	Joback Method
cpg	547.92	J/molxK	818.73	Joback Method
cpg	533.84	J/molxK	775.70	Joback Method
cpg	518.66	J/molxK	732.68	Joback Method
dvisc	0.0016009	Paxs	465.97	Joback Method
dvisc	0.0006851	Paxs	732.68	Joback Method
dvisc	0.0007540	Paxs	688.23	Joback Method
dvisc	0.0008408	Paxs	643.78	Joback Method
dvisc	0.0009529	Paxs	599.33	Joback Method
dvisc	0.0011019	Paxs	554.87	Joback Method
dvisc	0.0013067	Paxs	510.42	Joback Method
hfust	19.00	kJ/mol	390.70	NIST Webbook

## Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.40352e+01
Coeff. B	-5.59509e+03
Coeff. C	-1.44132e+02
Temperature range (K), min.	551.12
Temperature range (K), max.	785.50

## Sources

**NIST Webbook:**

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C3697243&Units=SI>

**The Yaws Handbook of Vapor**

<https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure>

**Pressure:  
Crippen Method:**

<http://pubs.acs.org/doi/abs/10.1021/ci9903071>

**Joback Method:**

[https://en.wikipedia.org/wiki/Joback\\_method](https://en.wikipedia.org/wiki/Joback_method)

**Aqueous Solubility Prediction Method:** <http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa>

**Estimated Solubility Method:** [http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl\\_file/ci034243xsi20040112\\_053635.txt](http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt)

**McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>

## 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>hfust:</b>	Enthalpy of fusion at a given temperature
<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>pvap:</b>	Vapor pressure
<b>rinpola:</b>	Non-polar retention indices
<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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