

# Pyrene, 1-phenyl-

<b>Other names:</b>	1-Phenylpyrene
<b>Inchi:</b>	InChI=1S/C22H14/c1-2-5-15(6-3-1)19-13-11-18-10-9-16-7-4-8-17-12-14-20(19)22(18)21
<b>InchiKey:</b>	QRVQUBKLRBKFCG-UHFFFAOYSA-N
<b>Formula:</b>	C22H14
<b>SMILES:</b>	c1ccc(-c2ccc3ccc4cccc5ccc2c3c45)cc1
<b>Mol. weight [g/mol]:</b>	278.35
<b>CAS:</b>	5101-27-9

## Physical Properties

Property code	Value	Unit	Source
gf	644.48	kJ/mol	Joback Method
hf	468.99	kJ/mol	Joback Method
hfus	33.69	kJ/mol	Joback Method
hvap	75.39	kJ/mol	Joback Method
log10ws	-8.90		Crippen Method
logp	6.251		Crippen Method
mcvol	219.240	ml/mol	McGowan Method
pc	2347.36	kPa	Joback Method
rinpol	457.93		NIST Webbook
rinpol	486.34		NIST Webbook
rinpol	457.93		NIST Webbook
rinpol	486.34		NIST Webbook
tb	820.30	K	Joback Method
tc	1089.89	K	Joback Method
tf	532.48	K	Joback Method
vc	0.848	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	607.64	J/molxK	820.30	Joback Method
cpg	622.45	J/molxK	865.23	Joback Method
cpg	636.52	J/molxK	910.16	Joback Method
cpg	650.13	J/molxK	955.09	Joback Method

cpg	663.56	J/mol×K	1000.03	Joback Method
cpg	677.10	J/mol×K	1044.96	Joback Method
cpg	691.04	J/mol×K	1089.89	Joback Method
dvisc	0.0022584	Paxs	532.48	Joback Method
dvisc	0.0019125	Paxs	580.45	Joback Method
dvisc	0.0016611	Paxs	628.42	Joback Method
dvisc	0.0014719	Paxs	676.39	Joback Method
dvisc	0.0013254	Paxs	724.36	Joback Method
dvisc	0.0012090	Paxs	772.33	Joback Method
dvisc	0.0011148	Paxs	820.30	Joback Method

## Sources

<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</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=C5101279&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C5101279&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>rinpol:</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

Latest version available from:

<https://www.cheméo.com/cid/16-573-8/Pyrene-1-phenyl.pdf>

Generated by Cheméo on 2024-04-27 05:37:18.624990905 +0000 UTC m=+16485487.545568224.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.