

# 1-Chloropyrene

<b>Other names:</b>	Pyrene, 1-chloro- 3-Chloropyrene
<b>Inchi:</b>	InChI=1S/C16H9Cl/c17-14-9-7-12-5-4-10-2-1-3-11-6-8-13(14)16(12)15(10)11/h1-9H
<b>InchiKey:</b>	WNYHOOQHJMHHQW-UHFFFAOYSA-N
<b>Formula:</b>	C16H9Cl
<b>SMILES:</b>	Clc1ccc2ccc3cccc4ccc1c2c34
<b>Mol. weight [g/mol]:</b>	236.70
<b>CAS:</b>	34244-14-9

## Physical Properties

Property code	Value	Unit	Source
gf	469.62	kJ/mol	Joback Method
hf	340.56	kJ/mol	Joback Method
hfus	28.30	kJ/mol	Joback Method
hvap	64.14	kJ/mol	Joback Method
log10ws	-6.99		Crippen Method
logp	5.237		Crippen Method
mcvol	170.700	ml/mol	McGowan Method
pc	2902.98	kPa	Joback Method
tb	693.77	K	Joback Method
tc	953.06	K	Joback Method
tf	392.15 ± 2.00	K	NIST Webbook
vc	0.668	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	408.64	J/mol×K	693.77	Joback Method
cpg	420.51	J/mol×K	736.98	Joback Method
cpg	431.47	J/mol×K	780.20	Joback Method
cpg	441.72	J/mol×K	823.41	Joback Method
cpg	451.48	J/mol×K	866.63	Joback Method
cpg	460.97	J/mol×K	909.84	Joback Method
cpg	470.39	J/mol×K	953.06	Joback Method

dvisc	0.0022260	Paxs	468.36	Joback Method
dvisc	0.0020098	Paxs	505.93	Joback Method
dvisc	0.0018405	Paxs	543.50	Joback Method
dvisc	0.0017047	Paxs	581.07	Joback Method
dvisc	0.0015937	Paxs	618.63	Joback Method
dvisc	0.0015014	Paxs	656.20	Joback Method
dvisc	0.0014237	Paxs	693.77	Joback Method

## Sources

<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</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=C34244149&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C34244149&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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