

# 1-Acetamidopyrene

<b>Other names:</b>	Acetamide, N-1-pyrenyl- N-Acetyl-1-aminopyrene N-1-Pyrenylacetamide
<b>Inchi:</b>	InChI=1S/C18H13NO/c1-11(20)19-16-10-8-14-6-5-12-3-2-4-13-7-9-15(16)18(14)17(12)1
<b>InchiKey:</b>	GJNGMQYHOZFNX-UHFFFAOYSA-N
<b>Formula:</b>	C18H13NO
<b>SMILES:</b>	CC(=O)Nc1ccc2ccc3cccc4ccc1c2c34
<b>Mol. weight [g/mol]:</b>	259.30
<b>CAS:</b>	22755-15-3

## Physical Properties

Property code	Value	Unit	Source
gf	458.86	kJ/mol	Joback Method
hf	255.91	kJ/mol	Joback Method
hfus	35.98	kJ/mol	Joback Method
hvap	77.39	kJ/mol	Joback Method
log10ws	-6.50		Crippen Method
logp	4.542		Crippen Method
mcvol	198.190	ml/mol	McGowan Method
pc	2670.78	kPa	Joback Method
tb	806.14	K	Joback Method
tc	1053.40	K	Joback Method
tf	563.57	K	Joback Method
vc	0.772	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	547.33	J/molxK	806.14	Joback Method
cpg	559.66	J/molxK	847.35	Joback Method
cpg	571.40	J/molxK	888.56	Joback Method
cpg	582.72	J/molxK	929.77	Joback Method
cpg	593.83	J/molxK	970.98	Joback Method
cpg	604.90	J/molxK	1012.19	Joback Method

## Sources

<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=C22755153&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C22755153&amp;Units=SI</a>
<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.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>

## Legend

<b>cpg:</b>	Ideal gas heat capacity
<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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