

# 1-Aminopyrene, TFA

<b>Inchi:</b>	InChI=1S/C18H10F3NO/c19-18(20,21)17(23)22-14-9-7-12-5-4-10-2-1-3-11-6-8-13(14)16
<b>InchiKey:</b>	IDPMQFBEJUQEGX-UHFFFAOYSA-N
<b>Formula:</b>	C18H10F3NO
<b>SMILES:</b>	O=C(Nc1ccc2ccc3cccc4ccc1c2c34)C(F)(F)F
<b>Mol. weight [g/mol]:</b>	313.27

## Physical Properties

Property code	Value	Unit	Source
gf	-122.73	kJ/mol	Joback Method
hf	-341.17	kJ/mol	Joback Method
hfus	37.81	kJ/mol	Joback Method
hvap	73.64	kJ/mol	Joback Method
log10ws	-7.17		Crippen Method
logp	5.085		Crippen Method
mcvol	203.500	ml/mol	McGowan Method
pc	2377.22	kPa	Joback Method
rinpol	413.72		NIST Webbook
rinpol	413.68		NIST Webbook
tb	800.72	K	Joback Method
tc	1031.37	K	Joback Method
tf	567.76	K	Joback Method
vc	0.816	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	572.35	J/mol×K	800.72	Joback Method
cpg	583.11	J/mol×K	839.16	Joback Method
cpg	593.32	J/mol×K	877.60	Joback Method
cpg	603.16	J/mol×K	916.05	Joback Method
cpg	612.83	J/mol×K	954.49	Joback Method
cpg	622.50	J/mol×K	992.93	Joback Method
cpg	632.37	J/mol×K	1031.37	Joback Method

# Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R537409&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R537409&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>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</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>hvp:</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>rinp:</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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