

# 5-Aminoacenaphthene TFA

<b>Inchi:</b>	InChI=1S/C14H10F3NO/c15-14(16,17)13(19)18-11-7-6-9-5-4-8-2-1-3-10(11)12(8)9/h1-3
<b>InchiKey:</b>	OYQLENJEYNMSST-UHFFFAOYSA-N
<b>Formula:</b>	C14H10F3NO
<b>SMILES:</b>	O=C(Nc1ccc2c3c(cccc13)CC2)C(F)(F)F
<b>Mol. weight [g/mol]:</b>	265.23

## Physical Properties

Property code	Value	Unit	Source
gf	-283.39	kJ/mol	Joback Method
hf	-495.99	kJ/mol	Joback Method
hfus	29.60	kJ/mol	Joback Method
hvap	62.15	kJ/mol	Joback Method
log10ws	-4.80		Crippen Method
logp	3.439		Crippen Method
mcvol	170.900	ml/mol	McGowan Method
pc	2676.31	kPa	Joback Method
rinpol	325.03		NIST Webbook
rinpol	324.22		NIST Webbook
tb	686.08	K	Joback Method
tc	905.12	K	Joback Method
tf	476.70	K	Joback Method
vc	0.683	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	463.63	J/mol×K	686.08	Joback Method
cpg	475.20	J/mol×K	722.59	Joback Method
cpg	485.87	J/mol×K	759.09	Joback Method
cpg	495.78	J/mol×K	795.60	Joback Method
cpg	505.05	J/mol×K	832.11	Joback Method
cpg	513.81	J/mol×K	868.61	Joback Method
cpg	522.18	J/mol×K	905.12	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=R537434&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R537434&amp;Units=SI</a>
<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>

# 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>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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