

# 2-Aminonaphthalene, TFA

<b>Inchi:</b>	InChI=1S/C12H8F3NO/c13-12(14,15)11(17)16-10-6-5-8-3-1-2-4-9(8)7-10/h1-7H,(H,16,17)
<b>InchiKey:</b>	LBQZDNKXORGQAD-UHFFFAOYSA-N
<b>Formula:</b>	C12H8F3NO
<b>SMILES:</b>	O=C(Nc1ccc2ccccc2c1)C(F)(F)F
<b>Mol. weight [g/mol]:</b>	239.19

## Physical Properties

Property code	Value	Unit	Source
gf	-361.53	kJ/mol	Joback Method
hf	-531.07	kJ/mol	Joback Method
hfus	26.03	kJ/mol	Joback Method
hvap	56.32	kJ/mol	Joback Method
log10ws	-4.14		Crippen Method
logp	3.341		Crippen Method
mcvol	153.580	ml/mol	McGowan Method
pc	2925.00	kPa	Joback Method
rinpol	285.69		NIST Webbook
rinpol	286.28		NIST Webbook
tb	623.22	K	Joback Method
tc	840.66	K	Joback Method
tf	403.42	K	Joback Method
vc	0.606	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	388.18	J/mol×K	623.22	Joback Method
cpg	400.05	J/mol×K	659.46	Joback Method
cpg	410.93	J/mol×K	695.70	Joback Method
cpg	420.89	J/mol×K	731.94	Joback Method
cpg	430.02	J/mol×K	768.18	Joback Method
cpg	438.42	J/mol×K	804.42	Joback Method
cpg	446.16	J/mol×K	840.66	Joback Method

# Sources

<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=R125294&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R125294&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>

# 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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