

# 4-Methyl-4-heptadecaneamine TFA

<b>Inchi:</b>	InChI=1S/C20H38F3NO/c1-4-6-7-8-9-10-11-12-13-14-15-17-19(3,16-5-2)24-18(25)20(21
<b>InchiKey:</b>	BCZZENCTJRBHLW-UHFFFAOYSA-N
<b>Formula:</b>	C20H38F3NO
<b>SMILES:</b>	CCCCCCCCCCCC(C)(CCC)NC(=O)C(F)(F)F
<b>Mol. weight [g/mol]:</b>	365.52

## Physical Properties

Property code	Value	Unit	Source
gf	-500.76	kJ/mol	Joback Method
hf	-1121.07	kJ/mol	Joback Method
hfus	48.67	kJ/mol	Joback Method
hvap	68.25	kJ/mol	Joback Method
log10ws	-7.93		Crippen Method
logp	6.925		Crippen Method
mcvol	309.520	ml/mol	McGowan Method
pc	1002.08	kPa	Joback Method
rinpol	2009.00		NIST Webbook
rinpol	2009.00		NIST Webbook
tb	752.39	K	Joback Method
tc	925.41	K	Joback Method
tf	424.36	K	Joback Method
vc	1.228	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	968.73	J/molxK	752.39	Joback Method
cpg	987.33	J/molxK	781.23	Joback Method
cpg	1004.96	J/molxK	810.06	Joback Method
cpg	1021.69	J/molxK	838.90	Joback Method
cpg	1037.58	J/molxK	867.74	Joback Method
cpg	1052.68	J/molxK	896.57	Joback Method
cpg	1067.05	J/molxK	925.41	Joback Method

# Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R571127&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R571127&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</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>

# 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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