

# Acetamide, N-[3-(10,11-dihydro-5H-dibenzo[a,d]cyclohepten-5

Other names:	Nortriptyline, TFA
Inchi:	InChI=1S/C21H20F3NO/c1-25(20(26)21(22,23)24)14-6-11-19-17-9-4-2-7-15(17)12-13-16
InchiKey:	UMONLFZBRKCYGG-UHFFFAOYSA-N
Formula:	C21H20F3NO
SMILES:	CN(CCC=C1c2ccccc2CCc2ccccc21)C(=O)C(F)(F)F
Mol. weight [g/mol]:	359.38
CAS:	55334-12-8

## Physical Properties

Property code	Value	Unit	Source
gf	-154.31	kJ/mol	Joback Method
hf	-499.61	kJ/mol	Joback Method
hfus	41.28	kJ/mol	Joback Method
hvap	74.27	kJ/mol	Joback Method
log10ws	-5.78		Crippen Method
logp	4.628		Crippen Method
mcvol	260.930	ml/mol	McGowan Method
pc	1645.76	kPa	Joback Method
tb	822.14	K	Joback Method
tc	1041.54	K	Joback Method
tf	523.44	K	Joback Method
vc	1.004	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	783.47	J/mol×K	822.14	Joback Method
cpg	798.40	J/mol×K	858.71	Joback Method
cpg	812.38	J/mol×K	895.27	Joback Method
cpg	825.55	J/mol×K	931.84	Joback Method
cpg	838.05	J/mol×K	968.41	Joback Method
cpg	850.04	J/mol×K	1004.97	Joback Method
cpg	861.64	J/mol×K	1041.54	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=C55334128&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C55334128&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.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>h vap:</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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