

# Dopamine, N-acetyl-TFA

<b>Other names:</b>	Dopamine, N-acetate, TFA
<b>Inchi:</b>	InChI=1S/C14H11F6NO5/c1-7(22)21-5-4-8-2-3-9(25-11(23)13(15,16)17)10(6-8)26-12(24)
<b>InchiKey:</b>	SFNUCMZHIIYINK-UHFFFAOYSA-N
<b>Formula:</b>	C14H11F6NO5
<b>SMILES:</b>	CC(=O)NCCc1ccc(OC(=O)C(F)(F)F)c(OC(=O)C(F)(F)F)c1
<b>Mol. weight [g/mol]:</b>	387.23

## Physical Properties

Property code	Value	Unit	Source
gf	-1510.40	kJ/mol	Joback Method
hf	-1861.57	kJ/mol	Joback Method
hfus	41.20	kJ/mol	Joback Method
hvap	74.36	kJ/mol	Joback Method
log10ws	-4.03		Crippen Method
logp	2.301		Crippen Method
mcvol	221.410	ml/mol	McGowan Method
pc	1849.92	kPa	Joback Method
rinpol	1588.00		NIST Webbook
rinpol	1588.00		NIST Webbook
rinpol	1588.00		NIST Webbook
tb	802.14	K	Joback Method
tc	995.74	K	Joback Method
tf	554.29	K	Joback Method
vc	0.886	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	655.28	J/molxK	802.14	Joback Method
cpg	665.07	J/molxK	834.41	Joback Method
cpg	674.05	J/molxK	866.67	Joback Method
cpg	682.25	J/molxK	898.94	Joback Method
cpg	689.70	J/molxK	931.21	Joback Method
cpg	696.46	J/molxK	963.47	Joback Method

## Sources

<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.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>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R57210&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R57210&amp;Units=SI</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>rinpol:</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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