

N-acetyltyramine-TFA

Other names:	Tyramine, N-acetate, TFA
Inchi:	InChI=1S/C12H12F3NO3/c1-8(17)16-7-6-9-2-4-10(5-3-9)19-11(18)12(13,14)15/h2-5H,6-
InchiKey:	DUWBWALLCDNSBT-UHFFFAOYSA-N
Formula:	C12H12F3NO3
SMILES:	CC(=O)NCCc1ccc(OC(=O)C(F)(F)F)cc1
Mol. weight [g/mol]:	275.22

Physical Properties

Property code	Value	Unit	Source
gf	-702.10	kJ/mol	Joback Method
hf	-966.94	kJ/mol	Joback Method
hfus	31.80	kJ/mol	Joback Method
hvap	63.84	kJ/mol	Joback Method
log10ws	-3.05		Crippen Method
logp	1.833		Crippen Method
mcpvol	180.480	ml/mol	McGowan Method
pc	2384.19	kPa	Joback Method
rinpol	1524.00		NIST Webbook
rinpol	1524.00		NIST Webbook
rinpol	1524.00		NIST Webbook
tb	680.53	K	Joback Method
tc	879.24	K	Joback Method
tf	442.88	K	Joback Method
vc	0.708	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	488.96	J/molxK	680.53	Joback Method
cpg	500.85	J/molxK	713.65	Joback Method
cpg	511.91	J/molxK	746.77	Joback Method
cpg	522.18	J/molxK	779.88	Joback Method
cpg	531.70	J/molxK	813.00	Joback Method
cpg	540.50	J/molxK	846.12	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R315932&Units=SI

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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