

N-Acetyltyramine

Other names:	Acetamide, N-[2-(4-hydroxyphenyl)ethyl]- N-(p-Hydroxyphenethyl) acetamide N-(2-(4-Hydroxyphenyl)ethyl)acetamide
Inchi:	InChI=1S/C10H13NO2/c1-8(12)11-7-6-9-2-4-10(13)5-3-9/h2-5,13H,6-7H2,1H3,(H,11,12)
InchiKey:	ATDWJOOPFDQZNK-UHFFFAOYSA-N
Formula:	C10H13NO2
SMILES:	CC(O)=NCCc1ccc(O)cc1
Mol. weight [g/mol]:	179.22
CAS:	1202-66-0

Physical Properties

Property code	Value	Unit	Source
hf	-270.31	kJ/mol	Joback Method
hvap	73.22	kJ/mol	Joback Method
log10ws	-1.64		Crippen Method
logp	1.911		Crippen Method
mcvol	145.420	ml/mol	McGowan Method
pc	3435.91	kPa	Joback Method
tb	704.24	K	Joback Method
tc	924.08	K	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1202660&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

hf:	Enthalpy of formation at standard conditions
h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀ws:	Log ₁₀ of Water solubility in mol/l
log_p:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature

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