Tyramine, N-formyl-

Other names: N-Formyltyramine
Inchi: InChI=1S/C9H11NO2/c11-7-10-6-5-8-1-3-9(12)4-2-8/h1-4,7,12H,5-6H2,(H,10,11)
InchiKey: ZRAJFHFOIYKZPF-UHFFFAOYSA-N
Formula: C9H11NO2
SMILES: OC=NCCc1ccc(O)cc1
Mol. weight [g/mol]: 165.19
CAS: 13062-78-7

Physical Properties

Property code	Value	Unit	Source
hf	-239.88	kJ/mol	Joback Method
hvap	70.91	kJ/mol	Joback Method
log10ws	-1.22		Crippen Method
logp	1.521		Crippen Method
mcvol	131.330	ml/mol	McGowan Method
pc	3834.03	kPa	Joback Method
rinpol	1882.10		NIST Webbook
rinpol	1882.10		NIST Webbook
tb	681.48	K	Joback Method
tc	901.55	K	Joback Method

Sources

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=C13062787&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

hf:	Enthalpy of formation 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