

2-(4-Acetyl-5-hydroxy-2-methoxyphenyl)ethylamine

Other names:	4-ethyl-2,5-dimethoxy-«beta»-phenethylamine-M, (O-desmethyl-oxo-N-acetyl)
Inchi:	InChI=1S/C13H17NO4/c1-8(15)11-7-13(18-3)10(6-12(11)17)4-5-14-9(2)16/h6-7,17H,4-5
InchiKey:	HWZXAJVKIWFYIF-UHFFFAOYSA-N
Formula:	C13H17NO4
SMILES:	COc1cc(C(C)=O)c(O)cc1CCNC(C)=O
Mol. weight [g/mol]:	251.28

Physical Properties

Property code	Value	Unit	Source
gf	-276.34	kJ/mol	Joback Method
hf	-579.28	kJ/mol	Joback Method
hfus	37.96	kJ/mol	Joback Method
hvap	83.48	kJ/mol	Joback Method
log10ws	-2.40		Crippen Method
logp	1.282		Crippen Method
mcvol	195.130	ml/mol	McGowan Method
pc	2787.66	kPa	Joback Method
rinpol	2320.00		NIST Webbook
rinpol	2320.00		NIST Webbook
tb	794.43	K	Joback Method
tc	1013.95	K	Joback Method
tf	574.20	K	Joback Method
vc	0.686	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	561.52	J/molxK	794.43	Joback Method
cpg	573.62	J/molxK	831.02	Joback Method
cpg	585.02	J/molxK	867.60	Joback Method
cpg	595.77	J/molxK	904.19	Joback Method
cpg	605.93	J/molxK	940.78	Joback Method
cpg	615.55	J/molxK	977.36	Joback Method
cpg	624.68	J/molxK	1013.95	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=U360339&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I

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
hvp:	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
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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