

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

Other names:	4-ethyl-2,5-dimethoxy-«beta»-phenethylamine-M, (O-desmethyl-oxo-N-acetyl), acetylated
Inchi:	INCHEM=1S/C15H19NO5/c1-9(17)13-8-14(20-4)12(5-6-16-10(2)18)7-15(13)21-11(3)19/h7-14
InchiKey:	CISVDWYZGPTYMJ-UHFFFAOYSA-N
Formula:	C15H19NO5
SMILES:	COc1cc(C(C)=O)c(OC(C)=O)cc1CCN=C(C)O
Mol. weight [g/mol]:	293.32

Physical Properties

Property code	Value	Unit	Source
hf	-720.21	kJ/mol	Joback Method
hvap	91.63	kJ/mol	Joback Method
log10ws	-3.19		Crippen Method
logp	2.342		Crippen Method
mcvol	224.880	ml/mol	McGowan Method
pc	1910.24	kPa	Joback Method
rinpol	2430.00		NIST Webbook
rinpol	2430.00		NIST Webbook
tb	905.54	K	Joback Method
tc	1120.71	K	Joback Method

Sources

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=U360340&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

hf: Enthalpy of formation at standard conditions

h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀ws:	Log10 of Water solubility in mol/l
log_p:	Octanol/Water partition coefficient
mc_{vol}:	McGowan's characteristic volume
p_c:	Critical Pressure
rin_{pol}:	Non-polar retention indices
t_b:	Normal Boiling Point Temperature
t_c:	Critical Temperature

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