4-Methoxyamphetamine, N-acetyl

Other names:	p-Methoxyamphetamine acetate
	N-Acetyl-p-methoxyamphetamine
Inchi:	InChI=1S/C12H17NO2/c1-9(13-10(2)14)8-11-4-6-12(15-3)7-5-11/h4-7,9H,8H2,1-3H3,(H,
InchiKey:	YGLMBIHCBHUNBV-UHFFFAOYSA-N
Formula:	C12H17NO2
SMILES:	COc1ccc(CC(C)N=C(C)O)cc1
Mol. weight [g/mol]:	207.27
CAS:	51920-74-2

Physical Properties

Property code	Value	Unit	Source
hf	-283.25	kJ/mol	Joback Method
hvap	67.34	kJ/mol	Joback Method
log10ws	-2.74		Crippen Method
logp	2.603		Crippen Method
mcvol	173.600	ml/mol	McGowan Method
pc	2331.52	kPa	Joback Method
rinpol	1720.00		NIST Webbook
rinpol	1720.00		NIST Webbook
tb	696.34	K	Joback Method
tc	903.86	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=C51920742&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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