1,3-Benzodioxol, 5-(acetylaminomethyl)

Inchi: InChI=1S/C10H11NO3/c1-7(12)11-5-8-2-3-9-10(4-8)14-6-13-9/h2-4H,5-6H2,1H3,(H,11,1
InchiKey: YFWYIWVJRPDXQD-UHFFFAOYSA-N
Formula: C10H11NO3
SMILES: CC(O)=NCc1ccc2c(c1)OCO2
Mol. weight [g/mol]: 193.20

Physical Properties

Property code	Value	Unit	Source
hf	-286.80	kJ/mol	Joback Method
hvap	70.77	kJ/mol	Joback Method
log10ws	-2.38		Crippen Method
logp	1.892		Crippen Method
mcvol	140.430	ml/mol	McGowan Method
pc	3302.95	kPa	Joback Method
rinpol	1940.00		NIST Webbook
tb	698.89	K	Joback Method
tc	921.20	K	Joback Method

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=R408856&Units=SI

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