

S(-)-Cathinone, N-acetyl-

Other names:	Acetamide, N-(1-benzoylethyl)
Inchi:	InChI=1S/C11H13NO2/c1-8(12-9(2)13)11(14)10-6-4-3-5-7-10/h3-8H,1-2H3,(H,12,13)
InchiKey:	XFOFGOGCAHRANZ-UHFFFAOYSA-N
Formula:	C11H13NO2
SMILES:	CC(O)=NC(C)C(=O)c1ccccc1
Mol. weight [g/mol]:	191.23

Physical Properties

Property code	Value	Unit	Source
hf	-231.50	kJ/mol	Joback Method
hvap	68.79	kJ/mol	Joback Method
log10ws	-2.48		Crippen Method
logp	2.234		Crippen Method
mcvol	155.210	ml/mol	McGowan Method
pc	2829.33	kPa	Joback Method
rinpol	1610.00		NIST Webbook
rinpol	1610.00		NIST Webbook
tb	699.93	K	Joback Method
tc	918.09	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=U353225&Units=SI

Legend

hf: Enthalpy of formation at standard conditions

h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀w_s:	Log10 of Water solubility in mol/l
log_p:	Octanol/Water partition coefficient
mc_{vol}:	McGowan's characteristic volume
p_c:	Critical Pressure
ri_{npol}:	Non-polar retention indices
t_b:	Normal Boiling Point Temperature
t_c:	Critical Temperature

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