Normephedrone, Ac

Inchi: InChI=1S/C12H15NO2/c1-8-4-6-11(7-5-8)12(15)9(2)13-10(3)14/h4-7,9H,1-3H3,(H,13,14)
InchiKey: VVDFFKRWYLPHEF-UHFFFAOYSA-N
Formula: C12H15NO2
SMILES: CC(O)=NC(C)C(=O)c1ccc(C)cc1
Mol. weight [g/mol]: 205.25

Physical Properties

Property code	Value	Unit	Source
hf	-263.61	kJ/mol	Joback Method
hvap	71.67	kJ/mol	Joback Method
log10ws	-2.96		Crippen Method
logp	2.543		Crippen Method
mcvol	169.300	ml/mol	McGowan Method
pc	2522.65	kPa	Joback Method
rinpol	1875.00		NIST Webbook
rinpol	1875.00		NIST Webbook
tb	727.79	K	Joback Method
tc	943.47	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=R615900&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

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