

Normethylone, Ac

Inchi:	InChI=1S/C12H13NO4/c1-7(13-8(2)14)12(15)9-3-4-10-11(5-9)17-6-16-10/h3-5,7H,6H2,1
InchiKey:	VZWRRVWZAVJEAP-UHFFFAOYSA-N
Formula:	C12H13NO4
SMILES:	CC(O)=NC(C)C(=O)c1ccc2c(c1)OCO2
Mol. weight [g/mol]:	235.24

Physical Properties

Property code	Value	Unit	Source
hf	-445.94	kJ/mol	Joback Method
hvap	81.58	kJ/mol	Joback Method
log10ws	-2.69		Crippen Method
logp	1.963		Crippen Method
mcvol	170.180	ml/mol	McGowan Method
pc	2887.40	kPa	Joback Method
rinpol	1930.00		NIST Webbook
rinpol	1930.00		NIST Webbook
tb	798.08	K	Joback Method
tc	1023.00	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=R615915&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
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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