

Methanone, bis(4-ethyl-3,5-dimethyl-1H-pyrrol-2-yl)-

Other names: Ketone, bis(4-ethyl-3,5-dimethylpyrrol-2-yl)
Inchi: InChI=1S/C17H24N2O/c1-7-13-9(3)15(18-11(13)5)17(20)16-10(4)14(8-2)12(6)19-16/h18
InchiKey: NAXHAHJDGRJNSQ-UHFFFAOYSA-N
Formula: C17H24N2O
SMILES: CCc1c(C)[nH]c(C(=O)c2[nH]c(C)c(CC)c2C)c1C
Mol. weight [g/mol]: 272.39
CAS: 13228-22-3

Physical Properties

Property code	Value	Unit	Source
chs	-9866.00 ± 10.00	kJ/mol	NIST Webbook
log10ws	-5.38		Crippen Method
logp	2.968		Crippen Method
mcvol	233.000	ml/mol	McGowan Method

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C13228223&Units=SI>

Legend

chs: Standard solid enthalpy of combustion
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume

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<https://www.chemeo.com/cid/20-545-4/Methanone-bis-4-ethyl-3-5-dimethyl-1H-pyrrol-2-yl.pdf>

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