1H-Pyrrole, 3-ethyl-5-[(4-ethyl-3,5-dimethyl-2H-pyrrol-2-yliden

Other names: Pyrrole, 3-ethyl-5-[(4-ethyl-3,5-dimethyl-2H-pyrrol-2-ylidene)methyl]-2,4-dimethyl-
2,2'-Dipyrromethene, 4,4'-diethyl-3,3',5,5'-tetramethyl-
3,5,3',5'-Tetramethyl-4,4'-diethyldipyrrylmethene
2H-Pyrrole, 4-ethyl-2-(4-ethyl-3,5-dimethyl-2-pyrrolylmethylene)-3,5-dimethyl-

Inchi: InChI=1S/C17H24N2/c1-7-14-10(3)16(18-12(14)5)9-17-11(4)15(8-2)13(6)19-17/h9,18H,7

InchiKey: QSPGBUOFJNDGBP-RQZCQDPDSA-N

Formula: C17H24N2

SMILES: CCC1=C(C)C(=Cc2[nH]c(C)c(CC)c2C)N=C1C

Mol. weight [g/mol]: 256.39

CAS: 2407-83-2

Physical Properties

Property code	Value	Unit	Source
chs	-10092.00 ± 10.00	kJ/mol	NIST Webbook
hfs	-27.00 ± 10.00	kJ/mol	NIST Webbook
log10ws	-5.61		Crippen Method
logp	4.254		Crippen Method
mcvol	227.130	ml/mol	McGowan Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2407832&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

chs: Standard solid enthalpy of combustion

hfs: Solid phase enthalpy of formation at standard conditions

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume