2,6-Dimethylbenzo-[1,2-d, 3,4-d]bisoxazole

Inchi: InChI=1S/C10H8N2O2/c1-5-11-7-3-4-8-9(10(7)14-5)12-6(2)13-8/h3-4H,1-2H3
InchiKey: DSKROQCUBLDQMB-UHFFFAOYSA-N
Formula: C10H8N2O2
SMILES: Cc1nc2c(ccc3nc(C)oc32)o1
Mol. weight [g/mol]: 188.18
CAS: 55850-41-4

Physical Properties

Property code	Value	Unit	Source
chs	-4865.90 ± 3.70	kJ/mol	NIST Webbook
log10ws	-13.03		Crippen Method
logp	2.586		Crippen Method
mcvol	129.380	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=C55850414&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
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.