2,7-Dimethylbenzo-[1,2-d,5,4-d]bisoxazole

Inchi: InChI=1S/C10H8N2O2/c1-5-11-7-3-8-10(4-9(7)13-5)14-6(2)12-8/h3-4H,1-2H3
InchiKey: JMLQVIGRGVEXEC-UHFFFAOYSA-N
Formula: C10H8N2O2
SMILES: Cc1nc2cc3nc(C)oc3cc2o1
Mol. weight [g/mol]: 188.18
CAS: 53816-93-6

Physical Properties

Property code	Value	Unit	Source
chs	-4870.90 ± 1.80	kJ/mol	NIST Webbook
log10ws	-13.03		Crippen Method
logp	2.586		Crippen Method
mcvol	129.380	ml/mol	McGowan Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C53816936&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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.