5-(1'-Formyl-2'-hydroxy-3'-naphthoylamino)-2-ben

Inchi: InChI=1S/C19H13N3O4/c23-9-14-12-4-2-1-3-10(12)7-13(17(14)24)18(25)20-11-5-6-15-1

InchiKey: XIOIVLSJFCJVLX-UHFFFAOYSA-N

Formula: C19H13N3O4

SMILES: O=Cc1c(O)c(C(O)=Nc2ccc3nc(O)[nH]c3c2)cc2ccccc12

Mol. weight [g/mol]: 347.32

CAS: 55447-62-6

Physical Properties

Property code	Value	Unit	Source
chs	-9087.50 ± 5.30	kJ/mol	NIST Webbook
hfs	-247.14	kJ/mol	NIST Webbook
log10ws	-5.09		Crippen Method
logp	3.094		Crippen Method
mcvol	241.250	ml/mol	McGowan Method

Sources

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=C55447626&Units=SI

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

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

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