1,2-Bis(phthalamido)benzene

Inchi: InChI=1S/C22H12N2O4/c25-19-13-7-1-2-8-14(13)20(26)23(19)17-11-5-6-12-18(17)24-21
InchiKey: QMYXYGOUFQPVGC-UHFFFAOYSA-N
Formula: C22H12N2O4
SMILES: O=C1c2ccccc2C(=O)N1c1ccccc1N1C(=O)c2ccccc2C1=O
Mol. weight [g/mol]: 368.34
CAS: 37881-98-4

Physical Properties

Property code	Value	Unit	Source
chs	-10004.00 ± 3.00	kJ/mol	NIST Webbook
hfs	-364.00	kJ/mol	NIST Webbook
log10ws	-5.65		Crippen Method
logp	3.288		Crippen Method
mcvol	254.080	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=C37881984&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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