Bis(3,4-bis(phthalamido)phenyl) ether

Inchi: InChI=1S/C44H22N4O9/c49-37-25-9-1-2-10-26(25)38(50)45(37)33-19-17-23(21-35(33)4
InchiKey: OWSUHASCUVBOBL-UHFFFAOYSA-N
Formula: C44H22N4O9
SMILES: O=C1c2ccccc2C(=O)N1c1ccc(Oc2ccc(N3C(=O)c4ccccc4C3=O)c(N3C(=O)c4ccccc4C3=
Mol. weight [g/mol]: 750.67
CAS: 52766-62-8

Physical Properties

Property code	Value	Unit	Source
chs	-19716.00 ± 2.00	kJ/mol	NIST Webbook
hfs	-742.70	kJ/mol	NIST Webbook
log10ws	-11.46		Crippen Method
logp	6.681		Crippen Method
mcvol	503.170	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=C52766628&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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