3,4-Dibenzamido-nitro-benzene

Inchi: InChI=1S/C20H15N3O4/c24-19(14-7-3-1-4-8-14)21-17-12-11-16(23(26)27)13-18(17)22-2
InchiKey: MTUBWAMJLNCCHT-UHFFFAOYSA-N
Formula: C20H15N3O4
SMILES: O=[N+]([O-])c1ccc(N=C(O)c2ccccc2)c(N=C(O)c2ccccc2)c1
Mol. weight [g/mol]: 361.35
CAS: 128049-26-3

Physical Properties

Property code	Value	Unit	Source
hf	60.16	kJ/mol	Joback Method
hvap	125.00	kJ/mol	Joback Method
log10ws	-5.49		Crippen Method
logp	4.867		Crippen Method
mcvol	261.900	ml/mol	McGowan Method
pc	2106.13	kPa	Joback Method
tb	1236.32	K	Joback Method
tc	1516.30	K	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C128049263&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Legend

hf: Enthalpy of formation at standard conditions
hvap: Enthalpy of vaporization at standard conditions
log10ws: Log10 of Water solubility in mol/l

logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature