4,4'-Biphenyldiisocyanate

Inchi: InChI=1S/C14H8N2O2/c17-9-15-13-5-1-11(2-6-13)12-3-7-14(8-4-12)16-10-18/h1-8H
InchiKey: RQBUVIFBALZGPC-UHFFFAOYSA-N
Formula: C14H8N2O2
SMILES: O=C=Nc1ccc(-c2ccc(N=C=O)cc2)cc1
Mol. weight [g/mol]: 236.23
CAS: 2761-22-0

Physical Properties

Property code	Value	Unit	Source
chs	-6602.40 ± 4.20	kJ/mol	NIST Webbook
hf	107.01	kJ/mol	Joback Method
hfs	-50.20 ± 4.20	kJ/mol	NIST Webbook
hvap	71.70	kJ/mol	Joback Method
log10ws	-13.04		Crippen Method
logp	3.288		Crippen Method
mcvol	175.100	ml/mol	McGowan Method
pc	3149.09	kPa	Joback Method
tb	716.38	K	Joback Method
tc	966.47	K	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2761220&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

chs: Standard solid enthalpy of combustion

hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase 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

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