1,5-Diisocyanatonaphthalene

Inchi: InChI=1S/C12H6N2O2/c15-7-13-11-5-1-3-9-10(11)4-2-6-12(9)14-8-16/h1-6H
InchiKey: SBJCUZQNHOLYMD-UHFFFAOYSA-N
Formula: C12H6N2O2
SMILES: O=C=Nc1cccc2c(N=C=O)cccc12
Mol. weight [g/mol]: 210.19

Physical Properties

Property code	Value	Unit	Source
hf	102.83	kJ/mol	Joback Method
hvap	66.61	kJ/mol	Joback Method
log10ws	-12.24		Crippen Method
logp	2.774		Crippen Method
mcvol	151.220	ml/mol	McGowan Method
pc	3560.02	kPa	Joback Method
tb	662.92	K	Joback Method
tc	905.69	K	Joback Method

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method: https://en.wikipedia.org/wiki/Joback_method
KDB: https://www.cheric.org/files/research/kdb/mol/mol1492.mol
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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