2-Methyl-1,5-naphthalene diisocyanate

Inchi: InChI=1S/C13H8N2O2/c1-9-5-6-10-11(13(9)15-8-17)3-2-4-12(10)14-7-16/h2-6H,1H3
InchiKey: WWWOJJNVCOVBNW-UHFFFAOYSA-N
Formula: C13H8N2O2
SMILES: Cc1ccc2c(N=C=O)cccc2c1N=C=O
Mol. weight [g/mol]: 224.21
CAS: 56775-58-7

Physical Properties

Property code	Value	Unit	Source
chs	-6125.40 ± 4.20	kJ/mol	NIST Webbook
hf	70.72	kJ/mol	Joback Method
hfs	-133.00 ± 4.20	kJ/mol	NIST Webbook
hvap	69.50	kJ/mol	Joback Method
log10ws	-12.72		Crippen Method
logp	3.083		Crippen Method
mcvol	165.310	ml/mol	McGowan Method
pc	3131.49	kPa	Joback Method
tb	690.78	K	Joback Method
tc	929.33	K	Joback Method

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C56775587&Units=SI

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