3-Nitraza-1,5-pentanediisocyanate

Inchi: InChI=1S/C6H8N4O4/c11-5-7-1-3-9(10(13)14)4-2-8-6-12/h1-4H2
InchiKey: PMZAXZNFRDOMGE-UHFFFAOYSA-N
Formula: C6H8N4O4
SMILES: O=C=NCCN(CCN=C=O)[N+](=O)[O-]
Mol. weight [g/mol]: 200.15
CAS: 7046-61-9

Physical Properties

Property code	Value	Unit	Source
chs	-3242.35	kJ/mol	NIST Webbook
hf	-121.22	kJ/mol	Joback Method
hfs	-142.10 ± 2.90	kJ/mol	NIST Webbook
hvap	66.65	kJ/mol	Joback Method
log10ws	-8.97		Crippen Method
logp	-0.848		Crippen Method
mcvol	137.300	ml/mol	McGowan Method
pc	3736.23	kPa	Joback Method
tb	634.30	K	Joback Method
tc	847.51	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=C7046619&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