o-Nitrosonitrobenzene dimer

Inchi: InChI=1S/C12H8N4O6/c17-13(9-5-1-3-7-11(9)15(19)20)14(18)10-6-2-4-8-12(10)16(21)2
InchiKey: LWSFKRORNVCQMT-BUHFOSPRSA-N
Formula: C12H8N4O6
SMILES: O=[N+]([O-])c1ccccc1[N+]([O-])=[N+]([O-])c1ccccc1[N+](=O)[O-]
Mol. weight [g/mol]: 304.22
CAS: 56079-22-2

Physical Properties

Property code	Value	Unit	Source
chs	-6082.00 ± 3.00	kJ/mol	NIST Webbook
hf	313.00 ± 4.00	kJ/mol	NIST Webbook
hfs	217.00 ± 3.00	kJ/mol	NIST Webbook
hsub	95.00 ± 1.00	kJ/mol	NIST Webbook
log10ws	-4.60		Crippen Method
logp	2.939		Crippen Method
mcvol	194.660	ml/mol	McGowan Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hsubt	95.50	kJ/mol	333.00	NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C56079222&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

chs:	Standard solid enthalpy of combustion
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation at standard conditions
hsub:	Enthalpy of sublimation at standard conditions
hsubt:	Enthalpy of sublimation at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume