Terephthalonitrile N,N'-dioxide

Other names: 1,4-Dicyanobenzene di-N-oxide
Inchi: InChI=1S/C8H4N2O2/c11-9-5-7-1-2-8(4-3-7)6-10-12/h1-4H
InchiKey: JRVRIUGIFUNROE-UHFFFAOYSA-N
Formula: C8H4N2O2
SMILES: [O-][N+]#Cc1ccc(C#[N+][O-])cc1
Mol. weight [g/mol]: 160.13
CAS: 3729-34-8

Physical Properties

Property code	Value	Unit	Source
chs	-4057.20 ± 1.50	kJ/mol	NIST Webbook
hf	410.50 ± 2.70	kJ/mol	NIST Webbook
hfs	337.50 ± 1.80	kJ/mol	NIST Webbook
hsub	73.00 ± 2.00	kJ/mol	NIST Webbook
hsub	73.00 ± 2.00	kJ/mol	NIST Webbook
log10ws	-8.88		Crippen Method
logp	2.044		Crippen Method
mcvol	114.320	ml/mol	McGowan Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C3729348&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume