2,4,6-Trinitropyridine 1-oxide

Inchi: InChI=1S/C5H2N4O7/c10-6-4(8(13)14)1-3(7(11)12)2-5(6)9(15)16/h1-2H
InchiKey: DQQZMAWSHWQSSF-UHFFFAOYSA-N
Formula: C5H2N4O7
SMILES: O=[N+]([O-])c1cc([N+](=O)[O-])[n+]([O-])c([N+](=O)[O-])c1
Mol. weight [g/mol]: 230.09
CAS: 25242-76-6

Physical Properties

Property code	Value	Unit	Source
chs	-2355.60 ± 1.30	kJ/mol	NIST Webbook
hfs	102.10 ± 1.30	kJ/mol	NIST Webbook
hsub	106.30 ± 2.90	kJ/mol	NIST Webbook
log10ws	-4.95		Crippen Method
logp	0.045		Crippen Method
mcvol	125.660	ml/mol	McGowan Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hsubt	106.30 ± 2.90	kJ/mol	390.00	NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C25242766&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Legend

chs:	Standard solid enthalpy of combustion
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