

Nitroguanylazide

Inchi: InChI=1S/CH2N6O2/c2-1(4-6-3)5-7(8)9/h(H2,2,5)
InchiKey: JGDWDXOANYXADQ-UHFFFAOYSA-N
Formula: CH2N6O2
SMILES: [N-]=[N+]=NC(N)=N[N+](=O)[O-]
Mol. weight [g/mol]: 130.07
CAS: 62154-79-4

Physical Properties

Property code	Value	Unit	Source
chs	-977.80 ± 4.30	kJ/mol	NIST Webbook
hfs	298.40 ± 4.30	kJ/mol	NIST Webbook
log10ws	-5.99		Crippen Method
logp	-0.197		Crippen Method
mcvol	79.370	ml/mol	McGowan Method

Sources

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>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C62154794&Units=SI>

Legend

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

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