2,4-DINITROSO-1,3-NAPHTHALENEDIOL

Other names: 1,3-Naphthalenediol, 2,4-dinitroso-
Inchi: InChI=1S/C10H6N2O4/c13-9-6-4-2-1-3-5(6)7(11-15)10(14)8(9)12-16/h1-4,13-14H
InchiKey: OCCDIVIHMBZDON-UHFFFAOYSA-N
Formula: C10H6N2O4
SMILES: O=Nc1c(O)c(N=O)c2ccccc2c1O
Mol. weight [g/mol]: 218.17

Physical Properties

Property code	Value	Unit	Source
hf	-72.76	kJ/mol	Cheméo Relay (1.0)
logp	3.047		Crippen Method
mcvol	143.380	ml/mol	McGowan Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C30436874&Units=SI
Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):

Legend

hf: Enthalpy of formation at standard conditions
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume