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
CAS: 30436-87-4

Physical Properties

Property code	Value	Unit	Source
hf	-536.07	kJ/mol	Joback Method
hvap	87.32	kJ/mol	Joback Method
log10ws	-3.89		Crippen Method
logp	3.047		Crippen Method
mcvol	143.380	ml/mol	McGowan Method
pc	5327.93	kPa	Joback Method
tb	771.86	K	Joback Method
tc	1014.31	K	Joback Method

Sources

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

Legend

hf: Enthalpy of formation at standard conditions
hvap: Enthalpy of vaporization at standard conditions

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature