2,5-dinitro-1H-imidazole

Inchi: InChI=1S/C3H2N4O4/c8-6(9)2-1-4-3(5-2)7(10)11/h1H,(H,4,5)
InchiKey: FLDSOXFRYVOGFK-UHFFFAOYSA-N
Formula: C3H2N4O4
SMILES: O=[N+]([O-])c1cnc([N+](=O)[O-])[nH]1
Mol. weight [g/mol]: 158.07

Physical Properties

Property code	Value	Unit	Source
hfus	6.64	kJ/mol	Thermal decomposition and kinetics of 2,4-dinitroimidazole: An insensitive high explosive
log10ws	-1.76		Crippen Method
logp	-0.256		Crippen Method
mcvol	88.470	ml/mol	McGowan Method
tt	501.15	K	Thermal decomposition and kinetics of 2,4-dinitroimidazole: An insensitive high explosive

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Thermal decomposition and kinetics of 2,4-dinitroimidazole: An insensitive high explosive: https://www.doi.org/10.1016/j.tca.2015.05.027
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

hfus: Enthalpy of fusion at standard conditions
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume

tt: Triple Point Temperature