5,7-DINITRO-8-HYDROXY-2-NAPHTHALENESULP ACID

Other names: 2,4-Dinitro-1-naphthol-7-sulfonic acid
2,4-Dinitronaphtholsulfonic acid
2-Naphthalenesulfonic acid, 5,7-dinitro-8-hydroxy-
2-Naphthalenesulfonic acid, 8-hydroxy-5,7-dinitro-
8-hydroxy-5,7-dinitronaphthalene-2-sulfonic acid
8-hydroxy-5,7-dinitronaphthalene-2-sulphonic acid
DNNS

Inchi: InChI=1S/C10H6N2O8S/c13-10-7-3-5(21(18,19)20)1-2-6(7)8(11(14)15)4-9(10)12(16)17/

InchiKey: FCQJEPASRCXVCB-UHFFFAOYSA-N

Formula: C10H6N2O8S

SMILES: O=[N+]([O-])c1cc([N+](=O)[O-])c2ccc(S(=O)(=O)O)cc2c1O

Mol. weight [g/mol]: 314.23

Physical Properties

Property code	Value	Unit	Source
hfus	55.52	kJ/mol	Joback Method
log10ws	-2.54		Aqueous Solubility Prediction Method
logp	1.609		Crippen Method
mcvol	183.210	ml/mol	McGowan Method
tf	516.27	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	521.67	J/mol×K	1013.06	Joback Method
cpg	528.34	J/mol×K	1055.86	Joback Method
cpg	534.83	J/mol×K	1098.65	Joback Method
cpg	541.29	J/mol×K	1141.45	Joback Method
cpg	547.83	J/mol×K	1184.24	Joback Method
cpg	554.57	J/mol×K	1227.04	Joback Method
cpg	561.63	J/mol×K	1269.83	Joback Method

Sources

Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C483841&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

Legend

cpg:	Ideal gas heat capacity
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
tf:	Normal melting (fusion) point