Flavianic 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

CAS: 483-84-1

Physical Properties

Property code	Value	Unit	Source
gf	-465.39	kJ/mol	Joback Method
hf	-660.95	kJ/mol	Joback Method
hfus	55.52	kJ/mol	Joback Method
hvap	125.27	kJ/mol	Joback Method
log10ws	-2.54		Aqueous Solubility Prediction Method
logp	1.609		Crippen Method
mcvol	183.210	ml/mol	McGowan Method
pc	6642.18	kPa	Joback Method
tb	1013.06	K	Joback Method
tc	1269.83	K	Joback Method
tf	797.46	K	Joback Method
vc	0.684	m3/kmol	Joback Method

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

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C483841&Units=SI

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion 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
tf:	Normal melting (fusion) point
vc:	Critical Volume