3-(4-Diethylamino-2-hydroxyphenylazo)-4-hydroxy acid

Other names: Benzenesulfonic acid, 3-((4-(diethylamino)-2-hydroxyphenyl)azo)-4-hydroxy-5-Sulfo-4'-(diethylamino)-2,2'-dihydroxyazobenzene

Inchi: InChI=1S/C16H19N3O5S/c1-3-19(4-2)11-5-7-13(16(21)9-11)17-18-14-10-12(25(22,23)24

InchiKey: DSZXUTUBVLAYLI-UHFFFAOYSA-N

Formula: C16H19N3O5S

SMILES: CCN(CC)c1ccc(N=Nc2cc(S(=O)(=O)O)ccc2O)c(O)c1

Mol. weight [g/mol]: 365.40

CAS: 1563-01-5

Physical Properties

Property code	Value	Unit	Source
hf	-768.90	kJ/mol	Joback Method
hvap	127.14	kJ/mol	Joback Method
log10ws	-2.94		Crippen Method
logp	3.606		Crippen Method
mcvol	260.120	ml/mol	McGowan Method
pc	2950.48	kPa	Joback Method
tb	1091.64	K	Joback Method
tc	1340.74	K	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1563015&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