P'-diethylamino-p-azobenzene sulfonic acid

Inchi: InChI=1S/C16H19N3O3S/c1-3-19(4-2)15-9-5-13(6-10-15)17-18-14-7-11-16(12-8-14)23(2
InchiKey: OORQUAGUOJMPCS-ISLYRVAYSA-N
Formula: C16H19N3O3S
SMILES: CCN(CC)c1ccc(N=Nc2ccc(S(=O)(=O)O)cc2)cc1
Mol. weight [g/mol]: 333.40
CAS: 6287-12-3

Physical Properties

Property code	Value	Unit	Source
hf	-414.28	kJ/mol	Joback Method
hvap	101.11	kJ/mol	Joback Method
log10ws	-3.85		Crippen Method
logp	4.195		Crippen Method
mcvol	248.380	ml/mol	McGowan Method
pc	2185.64	kPa	Joback Method
tb	930.40	K	Joback Method
tc	1156.58	K	Joback Method

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C6287123&Units=SI

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