

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

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

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