

Benzenamine, 4-methyl-N-sulfinyl-

Other names:	p-Toluidine, N-sulfinyl- p-Methyl-N-sulfinylaniline p-Tolylsulfinylamine N-Sulfinyl-p-toluidine Thionyl-p-toluidine 4-Methyl-N-sulfinylaniline 4-Methylsulfinylaniline 4-Methyl-N-sulfinylbenzenamine
Inchi:	InChI=1S/C7H7NOS/c1-6-2-4-7(5-3-6)8-10-9/h2-5H,1H3
InchiKey:	KLHMRBYLBVCGDT-UHFFFAOYSA-N
Formula:	C7H7NOS
SMILES:	<chem>Cc1ccc(N=S=O)cc1</chem>
Mol. weight [g/mol]:	153.20
CAS:	15795-42-3

Physical Properties

Property code	Value	Unit	Source
hf	-89.07	kJ/mol	Joback Method
hvap	50.03	kJ/mol	Joback Method
ie	8.84	eV	NIST Webbook
log10ws	-1.72		Crippen Method
logp	2.023		Crippen Method
mvol	113.630	ml/mol	McGowan Method
pc	4031.24	kPa	Joback Method
tb	523.40	K	Joback Method
tc	757.93	K	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C15795423&Units=SI

Legend

hf:	Enthalpy of formation at standard conditions
h_{vap}:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log₁₀ws:	Log10 of Water solubility in mol/l
log_p:	Octanol/Water partition coefficient
m_{cvol}:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature

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