

# Benzenesulfonyl isocyanate, 4-methyl-

<b>Other names:</b>	4-Methylbenzenesulfonyl isocyanate p-Methylphenylsulfonyl isocyanate 4-Methylphenylsulfonyl isocyanate p-Toluenesulfonic acid, anhydride with isocyanic acid p-Toluenesulfonyl isocyanate 4-Toluenesulfonyl isocyanate p-Tolylsulfonyl isocyanate Tosyl isocyanate p-Tosyl isocyanate 4-Isocyanatosulphonyltoluene, p-Toluensulfonyl isocyanate Sulfone, isocyanato tolyl p-Toluenesulphonyl isocyanate
<b>Inchi:</b>	InChI=1S/C8H7NO3S/c1-7-2-4-8(5-3-7)13(11,12)9-6-10/h2-5H,1H3
<b>InchiKey:</b>	VLJQDHDVZJXNQL-UHFFFAOYSA-N
<b>Formula:</b>	C8H7NO3S
<b>SMILES:</b>	<chem>Cc1ccc(S(=O)(=O)N=C=O)cc1</chem>
<b>Mol. weight [g/mol]:</b>	197.21
<b>CAS:</b>	4083-64-1

## Physical Properties

Property code	Value	Unit	Source
hf	-442.15	kJ/mol	Joback Method
hvap	64.51	kJ/mol	Joback Method
log10ws	-6.13		Crippen Method
logp	1.020		Crippen Method
mcvol	135.160	ml/mol	McGowan Method
pc	4815.84	kPa	Joback Method
tb	528.55	K	Joback Method
tc	742.59	K	Joback Method

## Sources

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C4083641&Units=SI>

**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci990307l>  
**Crippen Method:** [https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)  
**Joback Method:** [https://en.wikipedia.org/wiki/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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