4-Methylbenzenesulfonyl isocyanate

Other names:	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
Inchi:	InChI=1S/C8H7NO3S/c1-7-2-4-8(5-3-7)13(11,12)9-6-10/h2-5H,1H3
InchiKey:	VLJQDHDVZJXNQL-UHFFFAOYSA-N
Formula:	C8H7NO3S
SMILES:	Cc1ccc(S(=O)(=O)N=C=O)cc1
Mol. weight [g/mol]:	197.22

Physical Properties

Property code	Value	Unit	Source
hf	-310.40	kJ/mol	Cheméo Relay (1.0)
hvap	66.33	kJ/mol	Cheméo Relay (1.0)
ie	9.39	eV	Cheméo Relay (1.0)
log10ws	-2.85		Cheméo Relay (1.0)
logp	1.020		Crippen Method
mcvol	135.160	ml/mol	McGowan Method
tb	538.84	K	Cheméo Relay (1.0)
tf	360.37	K	Cheméo Relay (1.0)

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4083641&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	

Legend

hf:	Enthalpy of formation at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point