

Benzene, 1-isothiocyanato-4-methyl-

Other names:	1-Isothiocyanato-4-methylbenzene Isothiocyanic acid, p-tolyl ester p-Methylphenyl isothiocyanate 4-Methylphenyl isothiocyanate p-Tolyl isothiocyanate 4-Tolyl isothiocyanate Isothiocyanic acid, 4-tolyl ester
Inchi:	InChI=1S/C8H7NS/c1-7-2-4-8(5-3-7)9-6-10/h2-5H,1H3
InchiKey:	ABQKHKWXTUVKGF-UHFFFAOYSA-N
Formula:	C8H7NS
SMILES:	<chem>Cc1ccc(N=C=S)cc1</chem>
Mol. weight [g/mol]:	149.21
CAS:	622-59-3

Physical Properties

Property code	Value	Unit	Source
hf	300.68	kJ/mol	Joback Method
hvap	46.78	kJ/mol	Joback Method
log10ws	-2.87		Crippen Method
logp	2.729		Crippen Method
mcvol	117.550	ml/mol	McGowan Method
pc	3682.02	kPa	Joback Method
tb	560.05	K	Joback Method
tc	821.05	K	Joback Method

Sources

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=C622593&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

hf:	Enthalpy of formation at standard conditions
h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀ws:	Log ₁₀ of Water solubility in mol/l
log_p:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature

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