m-Tolyl isothiocyanate

Other names:	3-Methylphenyl isothiocyanate
	Benzene, 1-isothiocyanato-3-methyl-
Inchi:	InChI=1S/C8H7NS/c1-7-3-2-4-8(5-7)9-6-10/h2-5H,1H3
InchiKey:	BDPQUWSFKCFOST-UHFFFAOYSA-N
Formula:	C8H7NS
SMILES:	Cc1cccc(N=C=S)c1
Mol. weight [g/mol]:	149.21
CAS:	621-30-7

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

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C621307&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