Benzene, 1-isocyanato-2-methyl-

Other names:	Isocyanic acid, o-tolyl ester
	o-Methylphenyl isocyanate
	2-Methylphenyl isocyanate
	o-Toluene isocyanate
	o-Tolyl isocyanate
	2-Tolyl isocyanate
Inchi:	InChI=1S/C8H7NO/c1-7-4-2-3-5-8(7)9-6-10/h2-5H,1H3
InchiKey:	VAYMIYBJLRRIFR-UHFFFAOYSA-N
Formula:	C8H7NO
SMILES:	Cc1ccccc1N=C=O
Mol. weight [g/mol]:	133.15
CAS:	614-68-6

Physical Properties

Property code	Value	Unit	Source
hf	11.20	kJ/mol	Joback Method
hvap	45.87	kJ/mol	Joback Method
ie	8.70 ± 0.10	eV	NIST Webbook
log10ws	-6.43		Crippen Method
logp	1.962		Crippen Method
mcvol	107.070	ml/mol	McGowan Method
pc	3925.85	kPa	Joback Method
tb	480.77	K	Joback Method
tc	703.01	K	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C614686&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

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
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature