Benzene, 1-isocyanato-4-methyl-

Other names:	1-Isocyanato-4-methylbenzene
	4-Isocyanato-1-methylbenzene
	4-Isocyanatotoluene
	4-Methylphenyl isocyanate
	4-Tolyl isocyanate
	Isocyanic acid, p-tolyl ester
	p-Isocyanatotoluene
	p-Methylphenyl isocyanate
	p-Toluene isocyanate
	p-Tolyl isocyanate
Inchi:	InChI=1S/C8H7NO/c1-7-2-4-8(5-3-7)9-6-10/h2-5H,1H3
InchiKey:	MGYGFNQQGAQEON-UHFFFAOYSA-N
Formula:	C8H7NO
SMILES:	Cc1ccc(N=C=O)cc1
Mol. weight [g/mol]:	133.15
CAS:	622-58-2

Physical Properties

Property code	Value	Unit	Source
hf	11.20	kJ/mol	Joback Method
hvap	45.87	kJ/mol	Joback Method
ie	8.60 ± 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

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)

Coeff. A	8.75692e+00
Coeff. B	-1.75219e+03
Coeff. C	-3.54340e+01
Temperature range (K), min.	242.32
Temperature range (K), max.	543.99

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C622582&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

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
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature