Benzene, 1,3-diisocyanato-2-methyl-

Other names:	2,6-Diisocyanatotoluene
	Isocyanic acid, 2-methyl-m-phenylene ester
	2-Methyl-m-phenylene isocyanate
	2,6-TDI
	Toluene 2,6-Diisocyanate
	Tolylene 2,6-diisocyanate
	m-Tolylene diisocyanate
	2,6-Toluene diisocyanate
	2-Methyl-m-phenylene diisocyanate
	Benzene, 2,6-diisocyanato-1-methyl-
	2,6-Diisocyanato-1-methylbenzene
	Isocyanic acid, 2-methyl-meta-phenylene ester
	2-Methyl-meta-phenylene diisocyanate
	2-Methyl-meta-phenylene isocyanate
	meta-Tolylene diisocyanate
Inchi:	InChI=1S/C9H6N2O2/c1-7-8(10-5-12)3-2-4-9(7)11-6-13/h2-4H,1H3
InchiKey:	RUELTTOHQODFPA-UHFFFAOYSA-N
Formula:	C9H6N2O2
SMILES:	Cc1c(N=C=O)cccc1N=C=O
Mol. weight [g/mol]:	174.16
CAS:	91-08-7

Physical Properties

Property code	Value	Unit	Source
hf	-26.32	kJ/mol	Joback Method
hvap	58.29	kJ/mol	Joback Method
log10ws	-10.91		Crippen Method
logp	1.930		Crippen Method
mcvol	128.410	ml/mol	McGowan Method
pc	3749.97	kPa	Joback Method
tb	575.30	K	Joback Method
tc	802.50	K	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hvapt	60.40	kJ/mol	418.00	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C91087&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
hvapt:	Enthalpy of vaporization at a given temperature
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