m-Phenylene diisocyanate

Other names:	Benzene, 1,3-diisocyanato-
	m-Phenylene isocyanate
	Benzene 1,3-diisocyanate
	Benzene, m-diisocyanato-
	Isocyanic acid, m-phenylene ester
	Nacconate 400
	1,3-Diisocyanatobenzene
	1,3-Phenylene diisocyanate
	NSC 511721
Inchi:	InChI=1S/C8H4N2O2/c11-5-9-7-2-1-3-8(4-7)10-6-12/h1-4H
InchiKey:	VGHSXKTVMPXHNG-UHFFFAOYSA-N
Formula:	C8H4N2O2
SMILES:	O=C=Nc1cccc(N=C=O)c1
Mol. weight [g/mol]:	160.13
CAS:	123-61-5

Physical Properties

Property code	Value	Unit	Source
hf	5.79	kJ/mol	Joback Method
hvap	55.40	kJ/mol	Joback Method
log10ws	-10.44		Crippen Method
logp	1.621		Crippen Method
mcvol	114.320	ml/mol	McGowan Method
pc	4316.89	kPa	Joback Method
tb	547.44	K	Joback Method
tc	777.94	K	Joback Method

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=C123615&Units=SI

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