m-Xylylene diisocyanate

Other names:	Benzene, 1,3-bis(isocyanatomethyl)-
	Isocyanic acid, m-phenylenedimethylene ester
	1,3-Bis(isocyanatomethyl)benzene
	1,3-Bis-(isokyanatomethyl)benzen
	m-Phenylenedimethylene isocyanate
	Takenate
	Takenate 500
	M-Xdi
	m-Xylene diisocyanate
	m-Xylidene diisocyanate
	m-Xylylendiisokyanat
Inchi:	InChI=1S/C10H8N2O2/c13-7-11-5-9-2-1-3-10(4-9)6-12-8-14/h1-4H,5-6H2
InchiKey:	RTTZISZSHSCFRH-UHFFFAOYSA-N
Formula:	C10H8N2O2
SMILES:	O=C=NCc1cccc(CN=C=O)c1
Mol. weight [g/mol]:	188.18
CAS:	3634-83-1

Physical Properties

Property code	Value	Unit	Source
hf	-35.49	kJ/mol	Joback Method
hvap	59.86	kJ/mol	Joback Method
log10ws	-11.06		Crippen Method
logp	1.358		Crippen Method
mcvol	142.500	ml/mol	McGowan Method
pc	3403.91	kPa	Joback Method
tb	593.20	K	Joback Method
tc	815.17	K	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hvapt	46.70	kJ/mol	438.00	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3634831&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
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