

ALPHA,ALPHA'-DIISOCYANATO-M-XYLENE

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]:	188.19

Physical Properties

Property code	Value	Unit	Source
logp	1.358		Crippen Method
mcvol	142.500	ml/mol	McGowan Method
tb	541.73	K	Cheméo Relay (1.0)
tf	298.94	K	Cheméo Relay (1.0)

Temperature Dependent Properties

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

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3634831&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	

Legend

hvapt:	Enthalpy of vaporization at a given temperature
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point

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