Benzene, 2,4-diisocyanato-1-methyl- and benzene, 2,6-diisocyanato-1-methyl-

Inchi: InChI=1S/2C9H6N2O2/c1-7-2-3-8(5-10-12)4-9(7)6-11-13;1-7-8(5-10-12)3-2-4-9(7)6-11-1

InchiKey: PGMMANHWKICUSI-UHFFFAOYSA-N

Formula: C18H12N4O4

SMILES: Cc1c(C#[N+][O-])cccc1C#[N+][O-].Cc1ccc(C#[N+][O-])cc1C#[N+][O-]

Mol. weight [g/mol]: 348.31

Physical Properties

Property code	Value	Unit	Source
log10ws	-18.99		Crippen Method
logp	4.705		Crippen Method
mcvol	256.820	ml/mol	McGowan Method

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=B6010108&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume