

3,4,5-Trimethoxyphenyl isocyanate

Inchi: InChI=1S/C10H11NO4/c1-13-8-4-7(11-6-12)5-9(14-2)10(8)15-3/h4-5H,1-3H3
InchiKey: MJJXWPHZDBIHIM-UHFFFAOYSA-N
Formula: C10H11NO4
SMILES: COc1cc(N=C=O)cc(OC)c1OC
Mol. weight [g/mol]: 209.20

Physical Properties

Property code	Value	Unit	Source
logp	1.680		Crippen Method
mcvol	152.860	ml/mol	McGowan Method
tb	548.97	K	Cheméo Relay (1.0)

Sources

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.cheméo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C1016199&Units=SI>

Legend

logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
tb: Normal Boiling Point Temperature

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