

5-Chloro-2,4-dimethoxyphenyl isocyanate

Inchi: InChI=1S/C9H8ClNO3/c1-13-8-4-9(14-2)7(11-5-12)3-6(8)10/h3-4H,1-2H3
InchiKey: COSVEXSXJCUYOT-UHFFFAOYSA-N
Formula: C9H8ClNO3
SMILES: COc1cc(OC)c(N=C=O)cc1Cl
Mol. weight [g/mol]: 213.62
CAS: 55440-55-6

Physical Properties

Property code	Value	Unit	Source
hf	-312.56	kJ/mol	Joback Method
hvap	58.63	kJ/mol	Joback Method
log10ws	-6.88		Crippen Method
logp	2.325		Crippen Method
mcvol	145.140	ml/mol	McGowan Method
pc	3110.57	kPa	Joback Method
tb	595.88	K	Joback Method
tc	815.99	K	Joback Method

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307I>
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=C55440556&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

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