1-(Isocyanatomethyl)-4-(methyloxy)benzene

Inchi: InChI=1S/C9H9NO2/c1-12-9-4-2-8(3-5-9)6-10-7-11/h2-5H,6H2,1H3
InchiKey: QRBHVARIMDDOOV-UHFFFAOYSA-N
Formula: C9H9NO2
SMILES: COc1ccc(CN=C=O)cc1
Mol. weight [g/mol]: 163.17
CAS: 56651-60-6

Physical Properties

Property code	Value	Unit	Source
hf	-141.66	kJ/mol	Joback Method
hvap	50.51	kJ/mol	Joback Method
log10ws	-6.39		Crippen Method
logp	1.531		Crippen Method
mcvol	127.030	ml/mol	McGowan Method
pc	3423.86	kPa	Joback Method
rinpol	1385.50		NIST Webbook
rinpol	1385.50		NIST Webbook
tb	526.07	K	Joback Method
tc	742.38	K	Joback Method

Sources

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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C56651606&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature