Benzene, 1-isocyanato-4-methoxy-

Other names:	4-Methoxyphenylisocyanate
	p-Methoxyphenyl isocyanate
	p-Methoxyphenyl 1socyanate
	p-Anisyl isocyanate
	Isocyanic acid, p-methoxyphenyl ester
Inchi:	InChI=1S/C8H7NO2/c1-11-8-4-2-7(3-5-8)9-6-10/h2-5H,1H3
InchiKey:	FMDGXCSMDZMDHZ-UHFFFAOYSA-N
Formula:	C8H7NO2
SMILES:	COc1ccc(N=C=O)cc1
Mol. weight [g/mol]:	149.15
CAS:	5416-93-3

Physical Properties

Property code	Value	Unit	Source
hf	-121.02	kJ/mol	Joback Method
hvap	48.28	kJ/mol	Joback Method
log10ws	-6.07		Crippen Method
logp	1.662		Crippen Method
mcvol	112.940	ml/mol	McGowan Method
pc	3843.54	kPa	Joback Method
tb	503.19	K	Joback Method
tc	723.14	K	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5416933&Units=SI
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

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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