2-Methoxyphenyl isothiocyanate

Other names: Benzene, 1-isothiocyanato-2-methoxy-
o-Methoxyphenyl isothiocyanate
Inchi: InChI=1S/C8H7NOS/c1-10-8-5-3-2-4-7(8)9-6-11/h2-5H,1H3
InchiKey: QKAOOWJWWKWWOZ-UHFFFAOYSA-N
Formula: C8H7NOS
SMILES: COc1ccccc1N=C=S
Mol. weight [g/mol]: 165.21
CAS: 3288-04-8

Physical Properties

Property code	Value	Unit	Source
hf	168.46	kJ/mol	Joback Method
hvap	49.19	kJ/mol	Joback Method
log10ws	-2.51		Crippen Method
logp	2.429		Crippen Method
mcvol	123.420	ml/mol	McGowan Method
pc	3607.21	kPa	Joback Method
tb	582.47	K	Joback Method
tc	839.09	K	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C3288048&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