

4-Methoxyphenyl isothiocyanate

Other names:	Benzene, 1-isothiocyanato-4-methoxy- Phenylisothiocyanate, 4-methoxy p-methoxyphenyl isothiocyanate
Inchi:	InChI=1S/C8H7NOS/c1-10-8-4-2-7(3-5-8)9-6-11/h2-5H,1H3
InchiKey:	VRPQCVLBOZOYCG-UHFFFAOYSA-N
Formula:	C8H7NOS
SMILES:	<chem>COc1ccc(N=C=S)cc1</chem>
Mol. weight [g/mol]:	165.21
CAS:	2284-20-0

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

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=C2284200&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

hf:	Enthalpy of formation at standard conditions
h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀w_s:	Log ₁₀ of Water solubility in mol/l
log_p:	Octanol/Water partition coefficient
mc_{vol}:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature

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