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: COc1ccc(N=C=S)cc1
Mol. weight [g/mol]: 165.22

Physical Properties

Property code	Value	Unit	Source
hf	145.11	kJ/mol	Cheméo Relay (1.0)
hvap	64.70	kJ/mol	Cheméo Relay (1.0)
ie	7.92	eV	Cheméo Relay (1.0)
log10ws	-3.75		Cheméo Relay (1.0)
logp	2.429		Crippen Method
mcvol	123.420	ml/mol	McGowan Method
pc	3607.21	kPa	Joback Method
tb	512.87	K	Cheméo Relay (1.0)
tc	759.71	K	Cheméo Relay (1.0)
tf	315.85	K	Cheméo Relay (1.0)

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2284200&Units=SI
Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

hf:	Enthalpy of formation at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
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
tf:	Normal melting (fusion) point