4-Methoxy-2-methylphenyl isothiocyanate

Inchi: InChI=1S/C9H9NOS/c1-7-5-8(11-2)3-4-9(7)10-6-12/h3-5H,1-2H3
InchiKey: CXIJSTYYDYSTCX-UHFFFAOYSA-N
Formula: C9H9NOS
SMILES: COc1ccc(N=C=S)c(C)c1
Mol. weight [g/mol]: 179.24
CAS: 40046-28-4

Physical Properties

Property code	Value	Unit	Source
hf	136.35	kJ/mol	Joback Method
hvap	52.08	kJ/mol	Joback Method
log10ws	-2.99		Crippen Method
logp	2.738		Crippen Method
mcvol	137.510	ml/mol	McGowan Method
pc	3170.40	kPa	Joback Method
tb	610.33	K	Joback Method
tc	862.16	K	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C40046284&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

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