4-Methoxybenzoyl isothiocyanate

Inchi: InChI=1S/C9H7NO2S/c1-12-8-4-2-7(3-5-8)9(11)10-6-13/h2-5H,1H3
InchiKey: BEVJYGOHGKVXJI-UHFFFAOYSA-N
Formula: C9H7NO2S
SMILES: COc1ccc(C(=O)N=C=S)cc1
Mol. weight [g/mol]: 193.22
CAS: 16778-84-0

Physical Properties

Property code	Value	Unit	Source
hf	35.24	kJ/mol	Joback Method
hvap	58.16	kJ/mol	Joback Method
log10ws	-2.68		Crippen Method
logp	1.938		Crippen Method
mcvol	139.080	ml/mol	McGowan Method
pc	3468.36	kPa	Joback Method
tb	659.22	K	Joback Method
tc	916.43	K	Joback Method

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C16778840&Units=SI
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
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