3-Methoxycarbonylphenyl isothiocyanate

Inchi: InChI=1S/C9H7NO2S/c1-12-9(11)7-3-2-4-8(5-7)10-6-13/h2-5H,1H3
InchiKey: NQXFZEJJHPUMMF-UHFFFAOYSA-N
Formula: C9H7NO2S
SMILES: COC(=O)c1cccc(N=C=S)c1
Mol. weight [g/mol]: 193.22
CAS: 3125-66-4

Physical Properties

Property code	Value	Unit	Source
hf	35.24	kJ/mol	Joback Method
hvap	58.16	kJ/mol	Joback Method
log10ws	-2.63		Crippen Method
logp	2.208		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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C3125664&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