Methyl 2-isothiocyanato-3-phenylpropionate

Inchi: InChI=1S/C11H11NO2S/c1-14-11(13)10(12-8-15)7-9-5-3-2-4-6-9/h2-6,10H,7H2,1H3
InchiKey: XIAZBEQOUOVUEY-UHFFFAOYSA-N
Formula: C11H11NO2S
SMILES: COC(=O)C(Cc1ccccc1)N=C=S
Mol. weight [g/mol]: 221.28
CAS: 68521-58-4

Physical Properties

Property code	Value	Unit	Source
hf	0.15	kJ/mol	Joback Method
hvap	61.56	kJ/mol	Joback Method
log10ws	-2.44		Crippen Method
logp	1.873		Crippen Method
mcvol	167.260	ml/mol	McGowan Method
pc	2868.87	kPa	Joback Method
tb	699.56	K	Joback Method
tc	949.56	K	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C68521584&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