N-Phenethyl O-methyl thiocarbamate

Inchi: InChI=1S/C10H13NOS/c1-12-10(13)11-8-7-9-5-3-2-4-6-9/h2-6H,7-8H2,1H3,(H,11,13)
InchiKey: SABSUMPVZBKPRQ-UHFFFAOYSA-N
Formula: C10H13NOS
SMILES: COC(S)=NCCc1ccccc1
Mol. weight [g/mol]: 195.28
CAS: 930585-96-9

Physical Properties

Property code	Value	Unit	Source
hf	-34.51	kJ/mol	Joback Method
hvap	52.67	kJ/mol	Joback Method
log10ws	-2.43		Crippen Method
logp	2.161		Crippen Method
mcvol	155.900	ml/mol	McGowan Method
pc	2770.08	kPa	Joback Method
rinpol	1726.90		NIST Webbook
rinpol	1703.00		NIST Webbook
ripol	2827.00		NIST Webbook
tb	616.72	K	Joback Method
tc	861.88	K	Joback Method

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C930585969&Units=SI

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
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature