N-Phenethyl O-ethyl thiocarbamate

Inchi: InChI=1S/C11H15NOS/c1-2-13-11(14)12-9-8-10-6-4-3-5-7-10/h3-7H,2,8-9H2,1H3,(H,12,
InchiKey: XTJCUAOOXUKWRD-UHFFFAOYSA-N
Formula: C11H15NOS
SMILES: CCOC(S)=NCCc1ccccc1
Mol. weight [g/mol]: 209.31
CAS: 55365-88-3

Physical Properties

Property code	Value	Unit	Source
hf	-55.15	kJ/mol	Joback Method
hvap	54.90	kJ/mol	Joback Method
log10ws	-2.84		Crippen Method
logp	2.551		Crippen Method
mcvol	169.990	ml/mol	McGowan Method
pc	2510.03	kPa	Joback Method
rinpol	1773.00		NIST Webbook
ripol	2847.00		NIST Webbook
tb	639.60	K	Joback Method
tc	879.51	K	Joback Method

Sources

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=C55365883&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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