Isoxazole, 3-phenyl-

Other names: 3-Phenylisoxazole
Inchi: InChI=1S/C9H7NO/c1-2-4-8(5-3-1)9-6-7-11-10-9/h1-7H
InchiKey: ZBRDJMFLJXFIGJ-UHFFFAOYSA-N
Formula: C9H7NO
SMILES: c1ccc(-c2ccon2)cc1
Mol. weight [g/mol]: 145.16
CAS: 1006-65-1

Physical Properties

Property code	Value	Unit	Source
chl	-4617.50 ± 4.60	kJ/mol	NIST Webbook
hf	139.00 ± 6.30	kJ/mol	NIST Webbook
hfl	75.30 ± 4.60	kJ/mol	NIST Webbook
hvap	64.00 ± 4.20	kJ/mol	NIST Webbook
log10ws	-7.57		Crippen Method
logp	2.342		Crippen Method
mcvol	110.300	ml/mol	McGowan Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1006651&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Legend

chl: Standard liquid enthalpy of combustion
hf: Enthalpy of formation at standard conditions
hfl: Liquid phase 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