Isoxazole, 5-methyl-3-phenyl-

Other names: 5-Methyl-3-phenylisoxazole
Inchi: InChI=1S/C10H9NO/c1-8-7-10(11-12-8)9-5-3-2-4-6-9/h2-7H,1H3
InchiKey: UCGIIOJWRLQBRP-UHFFFAOYSA-N
Formula: C10H9NO
SMILES: Cc1cc(-c2ccccc2)no1
Mol. weight [g/mol]: 159.18
CAS: 1008-74-8

Physical Properties

Property code	Value	Unit	Source
chs	-5235.00 ± 5.40	kJ/mol	NIST Webbook
hf	98.70 ± 7.50	kJ/mol	NIST Webbook
hfl	14.00 ± 5.40	kJ/mol	NIST Webbook
hvap	84.90 ± 4.20	kJ/mol	NIST Webbook
log10ws	-8.05		Crippen Method
logp	2.650		Crippen Method
mcvol	124.390	ml/mol	McGowan Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1008748&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

chs: Standard solid 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