Isoxazole, 5-methyl-

Other names: NSC 52269
5-Methylisoxazole
Inchi: InChI=1S/C4H5NO/c1-4-2-3-5-6-4/h2-3H,1H3
InchiKey: AGQOIYCTCOEHGR-UHFFFAOYSA-N
Formula: C4H5NO
SMILES: Cc1ccno1
Mol. weight [g/mol]: 83.09
CAS: 5765-44-6

Physical Properties

Property code	Value	Unit	Source
chl	-2283.00 ± 0.71	kJ/mol	NIST Webbook
chl	-2261.70 ± 2.30	kJ/mol	NIST Webbook
hf	34.10 ± 0.75	kJ/mol	NIST Webbook
hf	15.00 ± 3.00	kJ/mol	NIST Webbook
hfl	-26.90 ± 2.30	kJ/mol	NIST Webbook
hfl	-5.61 ± 0.75	kJ/mol	NIST Webbook
hvap	39.70 ± 0.20	kJ/mol	NIST Webbook
hvap	42.00 ± 2.00	kJ/mol	NIST Webbook
hvap	39.70 ± 0.20	kJ/mol	NIST Webbook
ie	9.61	eV	NIST Webbook
log10ws	-5.45		Crippen Method
logp	0.983		Crippen Method
mcvol	63.610	ml/mol	McGowan Method
rinpol	702.00		NIST Webbook
rinpol	702.00		NIST Webbook
ripol	1215.00		NIST Webbook
ripol	1215.00		NIST Webbook
tb	395.20	K	NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C5765446&Units=SI

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

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
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature