2-Methylnaphth[2,3-d]oxazole

Other names:	2-methylnaphtho[2,3-d]oxazole
Inchi:	InChI=1S/C12H9NO/c1-8-13-11-6-9-4-2-3-5-10(9)7-12(11)14-8/h2-7H,1H3
InchiKey:	WMIHEWJRNFUVNR-UHFFFAOYSA-N
Formula:	C12H9NO
SMILES:	Cc1nc2cc3ccccc3cc2o1
Mol. weight [g/mol]:	183.21
CAS:	20686-66-2

Physical Properties

Property code	Value	Unit	Source
chs	-5955.90 ± 8.80	kJ/mol	NIST Webbook
log10ws	-9.06		Crippen Method
logp	3.289		Crippen Method
mcvol	137.410	ml/mol	McGowan Method
tf	359.27	K	Thermodynamic properties of naphthoxazole and naphthothiazole derivatives: Experimental and computational studies

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Thermodynamic properties of naphthoxazole and naphthothiazole derivatives: Experimental and computational studies:	https://www.doi.org/10.1016/j.jct.2018.07.008
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C20686662&Units=SI

Legend

chs:	Standard solid enthalpy of combustion
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient

mcvol:	McGowan's characteristic volume
tf:	Normal melting (fusion) point

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