

2,5-Dimethylbenzoxazole

Other names:	Benzoxazole, 2,5-dimethyl-
Inchi:	InChI=1S/C9H9NO/c1-6-3-4-9-8(5-6)10-7(2)11-9/h3-5H,1-2H3
InchiKey:	XVQGF GKAPKEUFT-UHFFFAOYSA-N
Formula:	C9H9NO
SMILES:	<chem>Cc1ccc2oc(C)nc2c1</chem>
Mol. weight [g/mol]:	147.18

Physical Properties

Property code	Value	Unit	Source
hf	-54.02	kJ/mol	Cheméo Relay (1.0)
log10ws	-2.39		Cheméo Relay (1.0)
logp	2.445		Crippen Method
mcvol	114.600	ml/mol	McGowan Method
tb	491.70	K	NIST Webbook
tf	305.34	K	Cheméo Relay (1.0)

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5676584&Units=SI
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	

Legend

hf:	Enthalpy of formation at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

tb: Normal Boiling Point Temperature

tf: Normal melting (fusion) point

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