2,5-Dimethylbenzoxalzole

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: XVQGFGKAPKEUFT-UHFFFAOYSA-N
Formula: C9H9NO
SMILES: Cc1ccc2oc(C)nc2c1
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.chemeo.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