3,6-Dimethyl-benzo-[b]-furan

Other names: 3,6-Dimethyl-benzo-[b]-furan
Benzofurane, 3,6-dimethyl
Inchi: InChI=1S/C10H10O/c1-7-3-4-9-8(2)6-11-10(9)5-7/h3-6H,1-2H3
InchiKey: VQIHEXZMNXLAFR-UHFFFAOYSA-N
Formula: C10H10O
SMILES: Cc1ccc2c(C)coc2c1
Mol. weight [g/mol]: 146.19

Physical Properties

Property code	Value	Unit	Source
hf	-39.84	kJ/mol	Cheméo Relay (1.0)
ie	8.01	eV	Cheméo Relay (1.0)
logp	3.050		Crippen Method
mcvol	118.710	ml/mol	McGowan Method
rinpol	1185.00		NIST Webbook
rinpol	1185.00		NIST Webbook
ripol	1730.00		NIST Webbook
tf	298.31	K	Cheméo Relay (1.0)

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C24410502&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

ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tf:	Normal melting (fusion) point