3-Phenylbenzo[b]furan

Other names: 3-Phenylbenzo[b]furan
Inchi: InChI=1S/C14H10O/c1-2-6-11(7-3-1)13-10-15-14-9-5-4-8-12(13)14/h1-10H
InchiKey: SSYBGLWXGRWEFE-UHFFFAOYSA-N
Formula: C14H10O
SMILES: c1ccc(-c2coc3ccccc23)cc1
Mol. weight [g/mol]: 194.23

Physical Properties

Property code	Value	Unit	Source
af	0.4479		Cheméo Relay (1.0)
hf	144.71	kJ/mol	Cheméo Relay (1.0)
hvap	85.83	kJ/mol	Cheméo Relay (1.0)
ie	7.97	eV	Cheméo Relay (1.0)
logp	4.100		Crippen Method
mcvol	151.310	ml/mol	McGowan Method
pc	3232.72	kPa	Cheméo Relay (1.0, beta)
tb	597.15	K	Cheméo Relay (1.0)
tc	872.08	K	Cheméo Relay (1.0)
tf	329.22	K	Cheméo Relay (1.0)
vc	0.584	m3/kmol	Cheméo Relay (1.0)

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C29909726&Units=SI
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

af:	Acentric Factor
hf:	Enthalpy of formation at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume