2-Benzoylfuran

Inchi: InChI=1S/C11H8O2/c12-11(10-7-4-8-13-10)9-5-2-1-3-6-9/h1-8H
InchiKey: CRLNTRZMHKNJSR-UHFFFAOYSA-N
Formula: C11H8O2
SMILES: O=C(c1ccccc1)c1ccco1
Mol. weight [g/mol]: 172.18

Physical Properties

Property code	Value	Unit	Source
af	0.4926		Cheméo Relay (1.0)
gf	-4.18	kJ/mol	Cheméo Relay (1.0, beta)
hf	-83.55	kJ/mol	Cheméo Relay (1.0)
hvap	79.15	kJ/mol	Cheméo Relay (1.0)
ie	9.10 ± 0.10	eV	NIST Webbook
log10ws	-2.79		Cheméo Relay (1.0)
logp	2.511		Crippen Method
mcvol	130.070	ml/mol	McGowan Method
pc	3533.89	kPa	Cheméo Relay (1.0, beta)
tb	558.20	K	NIST Webbook
tc	804.59	K	Cheméo Relay (1.0)
tf	302.30	K	Cheméo Relay (1.0)
vc	0.505	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=C2689590&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
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
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