3-Phenyl-2-benzofuranone

Inchi: InChI=1S/C14H10O2/c15-14-13(10-6-2-1-3-7-10)11-8-4-5-9-12(11)16-14/h1-9,13H
InchiKey: NANGQJICIOUURV-UHFFFAOYSA-N
Formula: C14H10O2
SMILES: O=C1Oc2ccccc2C1c1ccccc1
Mol. weight [g/mol]: 210.23
CAS: 3117-37-1

Physical Properties

Property code	Value	Unit	Source
gf	134.23	kJ/mol	Joback Method
hf	-67.60	kJ/mol	Joback Method
hfus	25.33	kJ/mol	Joback Method
hvap	60.64	kJ/mol	Joback Method
log10ws	-3.33		Crippen Method
logp	2.737		Crippen Method
mcvol	157.180	ml/mol	McGowan Method
pc	3231.98	kPa	Joback Method
tb	679.57	K	Joback Method
tc	947.36	K	Joback Method
tf	425.63	K	Joback Method
vc	0.589	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	413.79	J/mol×K	679.57	Joback Method
cpg	429.64	J/mol×K	724.20	Joback Method
cpg	444.09	J/mol×K	768.83	Joback Method
cpg	457.24	J/mol×K	813.47	Joback Method
cpg	469.16	J/mol×K	858.10	Joback Method
cpg	479.94	J/mol×K	902.73	Joback Method
cpg	489.67	J/mol×K	947.36	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3117371&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
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