3-(4-Hydroxyanilino)-2-benzofuran-1(3h)-one

Inchi: InChI=1S/C14H11NO3/c16-10-7-5-9(6-8-10)15-13-11-3-1-2-4-12(11)14(17)18-13/h1-8,1
InchiKey: WLBLNJAQWNYRGB-UHFFFAOYSA-N
Formula: C14H11NO3
SMILES: O=C1OC(Nc2ccc(O)cc2)c2ccccc21
Mol. weight [g/mol]: 241.24
CAS: 107558-84-9

Physical Properties

Property code	Value	Unit	Source
gf	69.00	kJ/mol	Joback Method
hf	-191.44	kJ/mol	Joback Method
hfus	36.21	kJ/mol	Joback Method
hvap	80.09	kJ/mol	Joback Method
log10ws	-3.32		Crippen Method
logp	2.673		Crippen Method
mcvol	173.030	ml/mol	McGowan Method
pc	3920.94	kPa	Joback Method
tb	810.36	K	Joback Method
tc	1078.51	K	Joback Method
tf	590.01	K	Joback Method
vc	0.590	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	509.42	J/mol×K	810.36	Joback Method
cpg	522.41	J/mol×K	855.05	Joback Method
cpg	534.50	J/mol×K	899.74	Joback Method
cpg	545.86	J/mol×K	944.43	Joback Method
cpg	556.65	J/mol×K	989.12	Joback Method
cpg	567.03	J/mol×K	1033.82	Joback Method
cpg	577.17	J/mol×K	1078.51	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C107558849&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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