Benzofuran-2-one, 4-amino-2,3-dihydro-

Inchi: InChI=1S/C8H7NO2/c9-6-2-1-3-7-5(6)4-8(10)11-7/h1-3H,4,9H2
InchiKey: YOFBHFZFZSNSGS-UHFFFAOYSA-N
Formula: C8H7NO2
SMILES: Nc1cccc2c1CC(=O)O2
Mol. weight [g/mol]: 149.15
CAS: 75990-99-7

Physical Properties

Property code	Value	Unit	Source
gf	35.83	kJ/mol	Joback Method
hf	-137.63	kJ/mol	Joback Method
hfus	19.49	kJ/mol	Joback Method
hvap	56.62	kJ/mol	Joback Method
log10ws	-1.28		Crippen Method
logp	0.730		Crippen Method
mcvol	106.380	ml/mol	McGowan Method
pc	4829.24	kPa	Joback Method
tb	597.79	K	Joback Method
tc	854.60	K	Joback Method
tf	431.61	K	Joback Method
vc	0.391	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	257.57	J/mol×K	597.79	Joback Method
cpg	268.87	J/mol×K	640.59	Joback Method
cpg	279.37	J/mol×K	683.39	Joback Method
cpg	289.08	J/mol×K	726.19	Joback Method
cpg	298.05	J/mol×K	768.99	Joback Method
cpg	306.31	J/mol×K	811.80	Joback Method
cpg	313.90	J/mol×K	854.60	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C75990997&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

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