3(2H)-Benzofuranone

Other names:	.beta.-coumaranone
	2H-3-Benzofuranone
	3-coumaranone
	Coumaran-3-one
	Coumaranone
	benzo[b]furan-3(2H)-one
	benzofuran-3(2H)-one
Inchi:	InChI=1S/C8H6O2/c9-7-5-10-8-4-2-1-3-6(7)8/h1-4H,5H2
InchiKey:	MGKPCLNUSDGXGT-UHFFFAOYSA-N
Formula:	C8H6O2
SMILES:	O=C1COc2ccccc21
Mol. weight [g/mol]:	134.13
CAS:	7169-34-8

Physical Properties

Property code	Value	Unit	Source
gf	-20.99	kJ/mol	Joback Method
hf	-159.95	kJ/mol	Joback Method
hfus	14.68	kJ/mol	Joback Method
hvap	45.32	kJ/mol	Joback Method
log10ws	-1.73		Crippen Method
logp	1.262		Crippen Method
mcvol	96.400	ml/mol	McGowan Method
pc	4559.21	kPa	Joback Method
ripol	2008.00		NIST Webbook
tb	520.28	K	Joback Method
tc	767.66	K	Joback Method
tf	335.83	K	Joback Method
vc	0.361	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	208.42	J/mol×K	520.28	Joback Method

cpg	220.19	J/mol×K	561.51	Joback Method
cpg	231.14	J/mol×K	602.74	Joback Method
cpg	241.30	J/mol×K	643.97	Joback Method
cpg	250.73	J/mol×K	685.20	Joback Method
cpg	259.45	J/mol×K	726.43	Joback Method
cpg	267.50	J/mol×K	767.66	Joback Method
hvapt	85.80	kJ/mol	298.15	Energetics of 2- and 3-coumaranone isomers: A combined calorimetric and computational study

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=C7169348&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Energetics of 2- and 3-coumaranone isomers: A combined calorimetric and computational study:	https://www.doi.org/10.1016/j.jct.2013.08.012

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
hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume