1(3H)-Isobenzofuranone

Other names:	1-Phthalanone
	2-Benzofuran-1(3h)-one
	2-Hydroxymethylbenzoic acid, «gamma»-lactone
	Phthalolactone
	phthalide
Inchi:	InChI=1S/C8H6O2/c9-8-7-4-2-1-3-6(7)5-10-8/h1-4H,5H2
InchiKey:	WNZQDUSMALZDQF-UHFFFAOYSA-N
Formula:	C8H6O2
SMILES:	O=C1OCc2ccccc21
Mol. weight [g/mol]:	134.13
CAS:	87-41-2

Physical Properties

Property code	Value	Unit	Source
gf	-20.99	kJ/mol	Joback Method
hf	-159.95	kJ/mol	Joback Method
hfs	-366.00	kJ/mol	NIST Webbook
hfus	14.68	kJ/mol	Joback Method
hvap	45.32	kJ/mol	Joback Method
log10ws	-2.07		Crippen Method
logp	1.357		Crippen Method
mcvol	96.400	ml/mol	McGowan Method
pc	4559.21	kPa	Joback Method
rinpol	231.37		NIST Webbook
rinpol	2000.00		NIST Webbook
rinpol	2021.00		NIST Webbook
ripol	2356.00		NIST Webbook
tb	563.20	K	NIST Webbook
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	250.73	J/mol×K	685.20	Joback Method
cpg	259.45	J/mol×K	726.43	Joback Method
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	267.50	J/mol×K	767.66	Joback Method
hvapt	88.40	kJ/mol	298.15	The effect of ketone groups on the energetic properties of phthalan derivatives
hvapt	59.30	kJ/mol	465.50	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C87412&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
The effect of ketone groups on the energetic properties of phthalan derivatives:	https://www.doi.org/10.1016/j.jct.2015.12.018
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
hfs:	Solid phase 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
rinpol:	Non-polar retention indices
ripol:	Polar retention indices

tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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