1(3H)-Isobenzofuranone, 6,7-dimethoxy-

Other names:	6,7-Dimethoxy-2-benzofuran-1(3H)-one
	6,7-Dimethoxyphthalide
	6,7-dimethoxy-3H-2-benzofuran-1-one
	Meconic lactone
	Meconin
	Meconine
	Mekonin
	NSC 35547
	Opianyl
	Phthalide, 6,7-dimethoxy-
Inchi:	InChI=1S/C10H10O4/c1-12-7-4-3-6-5-14-10(11)8(6)9(7)13-2/h3-4H,5H2,1-2H3
InchiKey:	ORFFGRQMMWVHIB-UHFFFAOYSA-N
Formula:	C10H10O4
SMILES:	COc1ccc2c(c1OC)C(=O)OC2
Mol. weight [g/mol]:	194.18
CAS:	569-31-3

Physical Properties

Property code	Value	Unit	Source
gf	-233.41	kJ/mol	Joback Method
hf	-488.61	kJ/mol	Joback Method
hfus	21.46	kJ/mol	Joback Method
hvap	55.92	kJ/mol	Joback Method
log10ws	-1.89		Aqueous Solubility Prediction Method
logp	1.374		Crippen Method
mcvol	136.320	ml/mol	McGowan Method
pc	3314.37	kPa	Joback Method
rinpol	1768.00		NIST Webbook
rinpol	1765.00		NIST Webbook
rinpol	1769.00		NIST Webbook
rinpol	1768.00		NIST Webbook
rinpol	1765.00		NIST Webbook
tb	620.84	K	Joback Method
tc	853.43	K	Joback Method
tf	374.90	K	Aqueous Solubility Prediction Method

vc	0.509	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	341.97	J/mol×K	620.84	Joback Method
cpg	354.90	J/mol×K	659.60	Joback Method
cpg	367.13	J/mol×K	698.37	Joback Method
cpg	378.63	J/mol×K	737.13	Joback Method
cpg	389.39	J/mol×K	775.90	Joback Method
cpg	399.40	J/mol×K	814.66	Joback Method
cpg	408.64	J/mol×K	853.43	Joback Method

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Joback Method: https://en.wikipedia.org/wiki/Joback_method

Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C569313&Units=SI

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

rinpol: Non-polar retention indices

tb: Normal Boiling Point Temperature

tc: Critical Temperature

tf: Normal melting (fusion) point

vc: Critical Volume