Isobenzofuran-1(3H)-one, 3,6,7-trimethoxy-

Other names: 3,6,7-Trimethoxyisobenzofuran-1(3H)-one
Inchi: InChI=1S/C11H12O5/c1-13-7-5-4-6-8(9(7)14-2)10(12)16-11(6)15-3/h4-5,11H,1-3H3
InchiKey: LQKGJNWATGCZSR-UHFFFAOYSA-N
Formula: C11H12O5
SMILES: COc1ccc2c(c1OC)C(=O)OC2OC
Mol. weight [g/mol]: 224.21
CAS: 91144-03-5

Physical Properties

Property code	Value	Unit	Source
gf	-337.70	kJ/mol	Joback Method
hf	-661.81	kJ/mol	Joback Method
hfus	26.31	kJ/mol	Joback Method
hvap	60.24	kJ/mol	Joback Method
log10ws	-2.27		Crippen Method
logp	1.519		Crippen Method
mcvol	156.280	ml/mol	McGowan Method
pc	2820.33	kPa	Joback Method
tb	661.47	K	Joback Method
tc	886.50	K	Joback Method
tf	457.13	K	Joback Method
vc	0.583	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	417.98	J/mol×K	661.47	Joback Method
cpg	432.00	J/mol×K	698.98	Joback Method
cpg	445.23	J/mol×K	736.48	Joback Method
cpg	457.65	J/mol×K	773.99	Joback Method
cpg	469.21	J/mol×K	811.49	Joback Method
cpg	479.89	J/mol×K	849.00	Joback Method
cpg	489.63	J/mol×K	886.50	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C91144035&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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