3(2H)-Benzofuranone, 4,6-dimethyl-

Other names: 4,6-Dimethyl-1-benzofuran-3(2H)-one
4,6-Dimethyl-3(2H)-benzofuranone
Inchi: InChI=1S/C10H10O2/c1-6-3-7(2)10-8(11)5-12-9(10)4-6/h3-4H,5H2,1-2H3
InchiKey: PRPSHVVAZDXSJJ-UHFFFAOYSA-N
Formula: C10H10O2
SMILES: Cc1cc(C)c2c(c1)OCC2=O
Mol. weight [g/mol]: 162.19
CAS: 20895-44-7

Physical Properties

Property code	Value	Unit	Source
gf	-23.41	kJ/mol	Joback Method
hf	-224.17	kJ/mol	Joback Method
hfus	19.08	kJ/mol	Joback Method
hvap	51.09	kJ/mol	Joback Method
log10ws	-2.68		Crippen Method
logp	1.879		Crippen Method
mcvol	124.580	ml/mol	McGowan Method
pc	3448.03	kPa	Joback Method
tb	576.00	K	Joback Method
tc	815.58	K	Joback Method
tf	383.41	K	Joback Method
vc	0.473	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	295.24	J/mol×K	576.00	Joback Method
cpg	308.52	J/mol×K	615.93	Joback Method
cpg	321.01	J/mol×K	655.86	Joback Method
cpg	332.72	J/mol×K	695.79	Joback Method
cpg	343.70	J/mol×K	735.72	Joback Method
cpg	353.95	J/mol×K	775.65	Joback Method
cpg	363.50	J/mol×K	815.58	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C20895447&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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