3,6-Dimethyl-benzo-[b]-furan-2(3H)-one

Inchi: InChI=1S/C10H10O2/c1-6-3-4-8-7(2)10(11)12-9(8)5-6/h3-5,7H,1-2H3
InchiKey: JSJKAEKKWQOCEZ-UHFFFAOYSA-N
Formula: C10H10O2
SMILES: Cc1ccc2c(c1)OC(=O)C2C
Mol. weight [g/mol]: 162.19

Physical Properties

Property code	Value	Unit	Source
gf	-21.49	kJ/mol	Joback Method
hf	-233.04	kJ/mol	Joback Method
hfus	20.54	kJ/mol	Joback Method
hvap	50.12	kJ/mol	Joback Method
log10ws	-2.50		Crippen Method
logp	2.018		Crippen Method
mcvol	124.580	ml/mol	McGowan Method
pc	3376.28	kPa	Joback Method
ripol	2116.00		NIST Webbook
ripol	2116.00		NIST Webbook
tb	566.35	K	Joback Method
tc	804.88	K	Joback Method
tf	366.65	K	Joback Method
vc	0.472	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	297.91	J/mol×K	566.35	Joback Method
cpg	311.96	J/mol×K	606.11	Joback Method
cpg	325.16	J/mol×K	645.86	Joback Method
cpg	337.54	J/mol×K	685.62	Joback Method
cpg	349.12	J/mol×K	725.37	Joback Method
cpg	359.91	J/mol×K	765.13	Joback Method
cpg	369.95	J/mol×K	804.88	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R326160&Units=SI
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

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