2,3,4,5,6-Pentamethylbenzophenone

Other names: 2,3,4,5,6-Pentamethyl benzopheneone
Inchi: InChI=1S/C18H20O/c1-11-12(2)14(4)17(15(5)13(11)3)18(19)16-9-7-6-8-10-16/h6-10H,1-
InchiKey: JFFVBXWGARSRSC-UHFFFAOYSA-N
Formula: C18H20O
SMILES: Cc1c(C)c(C)c(C(=O)c2ccccc2)c(C)c1C
Mol. weight [g/mol]: 252.35
CAS: 20386-33-8

Physical Properties

Property code	Value	Unit	Source
gf	148.43	kJ/mol	Joback Method
hf	-111.72	kJ/mol	Joback Method
hfus	30.11	kJ/mol	Joback Method
hvap	70.27	kJ/mol	Joback Method
log10ws	-5.81		Crippen Method
logp	4.460		Crippen Method
mcvol	218.530	ml/mol	McGowan Method
pc	1896.95	kPa	Joback Method
tb	743.37	K	Joback Method
tc	974.83	K	Joback Method
tf	457.99	K	Joback Method
vc	0.834	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	594.97	J/mol×K	743.37	Joback Method
cpg	611.49	J/mol×K	781.95	Joback Method
cpg	626.87	J/mol×K	820.52	Joback Method
cpg	641.16	J/mol×K	859.10	Joback Method
cpg	654.40	J/mol×K	897.68	Joback Method
cpg	666.63	J/mol×K	936.25	Joback Method
cpg	677.89	J/mol×K	974.83	Joback Method
dvisc	0.0007175	Pa×s	457.99	Joback Method

dvisc	0.0004697	Pa×s	505.55	Joback Method
dvisc	0.0003308	Pa×s	553.12	Joback Method
dvisc	0.0002462	Pa×s	600.68	Joback Method
dvisc	0.0001914	Pa×s	648.24	Joback Method
dvisc	0.0001540	Pa×s	695.81	Joback Method
dvisc	0.0001274	Pa×s	743.37	Joback Method

Sources

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=C20386338&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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