p-Methoxybutyrophenone

Other names:	4-Methoxybutyrophenone
	p-Methoxybutyrophenone
	1-Butanone, 1-(4-methoxyphenyl)-
	Butyrophenone, 4'-methoxy-
	1-(4-Methoxyphenyl)-1-butanone
Inchi:	InChI=1S/C11H14O2/c1-3-4-11(12)9-5-7-10(13-2)8-6-9/h5-8H,3-4H2,1-2H3
InchiKey:	JLCDSZXBELPBRD-UHFFFAOYSA-N
Formula:	C11H14O2
SMILES:	CCCC(=O)c1ccc(OC)cc1
Mol. weight [g/mol]:	178.23

Physical Properties

Property code	Value	Unit	Source
hf	-290.31	kJ/mol	Cheméo Relay (1.0)
hfus	20.69	kJ/mol	Joback Method
hvap	72.32	kJ/mol	Cheméo Relay (1.0)
ie	8.30 ± 0.20	eV	NIST Webbook
log10ws	-3.17		Cheméo Relay (1.0)
logp	2.678		Crippen Method
mcvol	149.530	ml/mol	McGowan Method
tb	543.74	K	Cheméo Relay (1.0)
tf	320.95	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	346.15	J/mol×K	559.03	Joback Method
cpg	360.31	J/mol×K	594.08	Joback Method
cpg	373.70	J/mol×K	629.14	Joback Method
cpg	386.36	J/mol×K	664.19	Joback Method
cpg	398.29	J/mol×K	699.24	Joback Method
cpg	409.50	J/mol×K	734.30	Joback Method
cpg	420.01	J/mol×K	769.35	Joback Method
dvisc	0.0017437	Pa×s	324.83	Joback Method

dvisc	0.0009957	Pa×s	363.86	Joback Method
dvisc	0.0006338	Pa×s	402.90	Joback Method
dvisc	0.0004369	Pa×s	441.93	Joback Method
dvisc	0.0003200	Pa×s	480.96	Joback Method
dvisc	0.0002455	Pa×s	520.00	Joback Method
dvisc	0.0001955	Pa×s	559.03	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4160514&Units=SI

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point