

4'-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
CAS:	4160-51-4

Physical Properties

Property code	Value	Unit	Source
gf	-89.40	kJ/mol	Joback Method
hf	-290.11	kJ/mol	Joback Method
hfus	20.69	kJ/mol	Joback Method
hvap	52.17	kJ/mol	Joback Method
ie	8.30 ± 0.20	eV	NIST Webbook
log10ws	-3.09		Crippen Method
logp	2.678		Crippen Method
mcvol	149.530	ml/mol	McGowan Method
pc	2735.42	kPa	Joback Method
tb	559.03	K	Joback Method
tc	769.35	K	Joback Method
tf	324.83	K	Joback Method
vc	0.568	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	346.15	J/molxK	559.03	Joback Method
cpg	360.31	J/molxK	594.08	Joback Method
cpg	373.70	J/molxK	629.14	Joback Method

cpg	386.36	J/molxK	664.19	Joback Method
cpg	398.29	J/molxK	699.24	Joback Method
cpg	409.50	J/molxK	734.30	Joback Method
cpg	420.01	J/molxK	769.35	Joback Method
dvisc	0.0017437	Paxs	324.83	Joback Method
dvisc	0.0009957	Paxs	363.86	Joback Method
dvisc	0.0006338	Paxs	402.90	Joback Method
dvisc	0.0004369	Paxs	441.93	Joback Method
dvisc	0.0003200	Paxs	480.96	Joback Method
dvisc	0.0002455	Paxs	520.00	Joback Method
dvisc	0.0001955	Paxs	559.03	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=C4160514&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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
h vap:	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
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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