Isopropyl phenyl ketone

Other names:	1-Propanone, 2-methyl-1-phenyl- Isobutyrophenone «alpha»-Methylpropiophenone Phenyl isopropyl ketone 2-Methylpropiophenone 2-Methyl-1-phenyl-1-propanone
Inchi:	InChI=1S/C10H12O/c1-8(2)10(11)9-6-4-3-5-7-9/h3-8H,1-2H3
InchiKey:	BSMGLVDZZMBWQB-UHFFFAOYSA-N
Formula:	C10H12O
SMILES:	CC(C)C(=O)c1ccccc1
Mol. weight [g/mol]:	148.20
CAS:	611-70-1

Physical Properties

Property code	Value	Unit	Source
basg	839.30	kJ/mol	NIST Webbook
gf	14.37	kJ/mol	Joback Method
hf	-131.06	kJ/mol	Joback Method
hfus	13.77	kJ/mol	Joback Method
hvap	46.49	kJ/mol	Joback Method
log10ws	-2.73		Crippen Method
logp	2.525		Crippen Method
mcvol	129.570	ml/mol	McGowan Method
pc	3170.40	kPa	Joback Method
rinpol	1185.00		NIST Webbook
rinpol	1174.00		NIST Webbook
rinpol	1185.00		NIST Webbook
tb	490.20	K	NIST Webbook
tc	728.18	K	Joback Method
tf	263.81	K	Joback Method
vc	0.487	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	276.87	J/mol×K	508.31	Joback Method
cpg	339.99	J/mol×K	691.53	Joback Method
cpg	329.01	J/mol×K	654.89	Joback Method
cpg	317.24	J/mol×K	618.24	Joback Method
cpg	304.66	J/mol×K	581.60	Joback Method
cpg	291.21	J/mol×K	544.95	Joback Method
cpg	350.22	J/mol×K	728.18	Joback Method
dvisc	0.0002449	Pa×s	508.31	Joback Method
dvisc	0.0003205	Pa×s	467.56	Joback Method
dvisc	0.0004416	Pa×s	426.81	Joback Method
dvisc	0.0006510	Pa×s	386.06	Joback Method
dvisc	0.0010518	Pa×s	345.31	Joback Method
dvisc	0.0019321	Pa×s	304.56	Joback Method
dvisc	0.0042828	Pa×s	263.81	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	493.20	K	99.50	NIST Webbook
tbrp	359.20	K	0.50	NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C611701&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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Legend

basg: Gas basicity
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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume