p-Isobutylacetophenone

Other names:	p-iso-Butylacetophenone
	4-Isobutylacetophenone
	Ethanone, 1-[4-(2-methylpropyl)phenyl]-
	Acetophenone, 4-isobutyl-
	4'-Isobutylacetophenone
	1-[4-(2-methylpropyl)phenyl]ethan-1-one
Inchi:	InChI=1S/C12H16O/c1-9(2)8-11-4-6-12(7-5-11)10(3)13/h4-7,9H,8H2,1-3H3
InchiKey:	KEAGRYYGYWZVPC-UHFFFAOYSA-N
Formula:	C12H16O
SMILES:	CC(=O)c1ccc(CC(C)C)cc1
Mol. weight [g/mol]:	176.26

Physical Properties

Property code	Value	Unit	Source
af	0.5263		Cheméo Relay (1.0)
gf	21.58	kJ/mol	Joback Method
hf	-211.27	kJ/mol	Cheméo Relay (1.0)
hfus	18.56	kJ/mol	Joback Method
hvap	71.54	kJ/mol	Cheméo Relay (1.0)
ie	9.09	eV	Cheméo Relay (1.0)
log10ws	-3.66		Cheméo Relay (1.0)
logp	3.088		Crippen Method
mcvol	157.750	ml/mol	McGowan Method
pc	2543.05	kPa	Joback Method
rinpol	1411.00		NIST Webbook
tb	535.68	K	Cheméo Relay (1.0)
tc	736.44	K	Cheméo Relay (1.0)
tf	299.17	K	Cheméo Relay (1.0)
vc	0.577	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	368.69	J/mol×K	559.05	Joback Method

cpg	449.59	J/mol×K	772.73	Joback Method
cpg	438.16	J/mol×K	737.11	Joback Method
cpg	425.95	J/mol×K	701.50	Joback Method
cpg	412.94	J/mol×K	665.89	Joback Method
cpg	399.08	J/mol×K	630.28	Joback Method
cpg	384.34	J/mol×K	594.66	Joback Method
dvisc	0.0005236	Pa×s	428.96	Joback Method
dvisc	0.0002075	Pa×s	559.05	Joback Method
dvisc	0.0002682	Pa×s	515.69	Joback Method
dvisc	0.0003634	Pa×s	472.32	Joback Method
dvisc	0.0029584	Pa×s	298.87	Joback Method
dvisc	0.0008191	Pa×s	385.60	Joback Method
dvisc	0.0014350	Pa×s	342.23	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	407.50 ± 0.50	K	2.10	NIST Webbook

Sources

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=C38861788&Units=SI
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

Legend

af: Acentric Factor
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
ie:	Ionization energy
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