Benzyl isobutyl ketone

Other names: 2-Pentanone, 4-methyl-1-phenyl-
4-Methyl-1-phenyl-2-pentanone
4-methyl-1-phenylpentan-2-one
Inchi: InChI=1S/C12H16O/c1-10(2)8-12(13)9-11-6-4-3-5-7-11/h3-7,10H,8-9H2,1-2H3
InchiKey: DTYGTEGDVPAKDA-UHFFFAOYSA-N
Formula: C12H16O
SMILES: CC(C)CC(=O)Cc1ccccc1
Mol. weight [g/mol]: 176.25
CAS: 5349-62-2

Physical Properties

Property code	Value	Unit	Source
gf	31.21	kJ/mol	Joback Method
hf	-172.34	kJ/mol	Joback Method
hfus	18.95	kJ/mol	Joback Method
hvap	50.94	kJ/mol	Joback Method
log10ws	-2.99		Crippen Method
logp	2.844		Crippen Method
mcvol	157.750	ml/mol	McGowan Method
pc	2581.96	kPa	Joback Method
tb	523.70	K	NIST Webbook
tc	766.69	K	Joback Method
tf	286.35	K	Joback Method
vc	0.600	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	368.74	J/mol×K	554.07	Joback Method
cpg	384.70	J/mol×K	589.51	Joback Method
cpg	399.69	J/mol×K	624.94	Joback Method
cpg	413.76	J/mol×K	660.38	Joback Method
cpg	426.95	J/mol×K	695.82	Joback Method
cpg	439.29	J/mol×K	731.25	Joback Method

cpg	450.82	J/mol×K	766.69	Joback Method
dvisc	0.0041343	Pa×s	286.35	Joback Method
dvisc	0.0018071	Pa×s	330.97	Joback Method
dvisc	0.0009615	Pa×s	375.59	Joback Method
dvisc	0.0005850	Pa×s	420.21	Joback Method
dvisc	0.0003915	Pa×s	464.83	Joback Method
dvisc	0.0002811	Pa×s	509.45	Joback Method
dvisc	0.0002129	Pa×s	554.07	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	395.20	K	2.00	NIST Webbook

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=C5349622&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

tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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