1-Butanone, 3-methyl-1-phenyl-

Other names: 3-Methyl-1-phenyl-1-butanone
Isovalerophenone
Isobutyl phenyl ketone
1-Phenyl-3-methyl-1-butanone
Inchi: InChI=1S/C11H14O/c1-9(2)8-11(12)10-6-4-3-5-7-10/h3-7,9H,8H2,1-2H3
InchiKey: HEOVGVNITGAUKL-UHFFFAOYSA-N
Formula: C11H14O
SMILES: CC(C)CC(=O)c1ccccc1
Mol. weight [g/mol]: 162.23
CAS: 582-62-7

Physical Properties

Property code	Value	Unit	Source
gf	22.79	kJ/mol	Joback Method
hf	-160.70 ± 2.30	kJ/mol	NIST Webbook
hfl	-220.20 ± 1.50	kJ/mol	NIST Webbook
hfus	16.36	kJ/mol	Joback Method
hvap	59.50 ± 1.70	kJ/mol	NIST Webbook
hvap	59.50	kJ/mol	NIST Webbook
log10ws	-3.15		Crippen Method
logp	2.915		Crippen Method
mcvol	143.660	ml/mol	McGowan Method
pc	2853.57	kPa	Joback Method
rinpol	1271.00		NIST Webbook
tb	509.70	K	NIST Webbook
tc	747.39	K	Joback Method
tf	275.08	K	Joback Method
vc	0.543	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	399.97	J/mol×K	747.39	Joback Method
cpg	389.04	J/mol×K	711.36	Joback Method

cpg	377.33	J/mol×K	675.32	Joback Method
cpg	364.80	J/mol×K	639.29	Joback Method
cpg	351.41	J/mol×K	603.26	Joback Method
cpg	337.13	J/mol×K	567.22	Joback Method
cpg	321.92	J/mol×K	531.19	Joback Method
dvisc	0.0042401	Pa×s	275.08	Joback Method
dvisc	0.0002296	Pa×s	531.19	Joback Method
dvisc	0.0003019	Pa×s	488.51	Joback Method
dvisc	0.0004183	Pa×s	445.82	Joback Method
dvisc	0.0006210	Pa×s	403.14	Joback Method
dvisc	0.0010123	Pa×s	360.45	Joback Method
dvisc	0.0018817	Pa×s	317.77	Joback Method
hvapt	55.70	kJ/mol	416.00	NIST Webbook

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C582627&Units=SI

Legend

cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
gf: Standard Gibbs free energy of formation
hf: Enthalpy of formation at standard conditions
hfl: Liquid phase enthalpy of formation at standard conditions
hfus: Enthalpy of fusion at standard conditions
hvap: Enthalpy of vaporization at standard conditions
hvapt: Enthalpy of vaporization at a given temperature
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

tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume