1-Butanone, 2-methyl-1-phenyl-

Other names: «alpha»-Methylpropyl phenyl ketone
Inchi: InChI=1S/C11H14O/c1-3-9(2)11(12)10-7-5-4-6-8-10/h4-9H,3H2,1-2H3
InchiKey: DGZJLMWKIQOQFA-UHFFFAOYSA-N
Formula: C11H14O
SMILES: CCC(C)C(=O)c1ccccc1
Mol. weight [g/mol]: 162.23
CAS: 938-87-4

Physical Properties

Property code	Value	Unit	Source
gf	22.79	kJ/mol	Joback Method
hf	-151.70	kJ/mol	Joback Method
hfus	16.36	kJ/mol	Joback Method
hvap	48.71	kJ/mol	Joback Method
log10ws	-3.15		Crippen Method
logp	2.915		Crippen Method
mcvol	143.660	ml/mol	McGowan Method
pc	2853.57	kPa	Joback Method
rinpol	1262.00		NIST Webbook
tb	531.19	K	Joback Method
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	321.92	J/mol×K	531.19	Joback Method
cpg	337.13	J/mol×K	567.22	Joback Method
cpg	351.41	J/mol×K	603.26	Joback Method
cpg	364.80	J/mol×K	639.29	Joback Method
cpg	377.33	J/mol×K	675.32	Joback Method
cpg	389.04	J/mol×K	711.36	Joback Method
cpg	399.97	J/mol×K	747.39	Joback Method

dvisc	0.0042401	Pa×s	275.08	Joback Method
dvisc	0.0018817	Pa×s	317.77	Joback Method
dvisc	0.0010123	Pa×s	360.45	Joback Method
dvisc	0.0006210	Pa×s	403.14	Joback Method
dvisc	0.0004183	Pa×s	445.82	Joback Method
dvisc	0.0003019	Pa×s	488.51	Joback Method
dvisc	0.0002296	Pa×s	531.19	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C938874&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

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