1-Phenyl-2-butanone

Other names: Benzyl ethyl ketone
2-Butanone, 1-phenyl-
1-phenylbutan-2-one
Inchi: InChI=1S/C10H12O/c1-2-10(11)8-9-6-4-3-5-7-9/h3-7H,2,8H2,1H3
InchiKey: GKDLTXYXODKDEA-UHFFFAOYSA-N
Formula: C10H12O
SMILES: CCC(=O)Cc1ccccc1
Mol. weight [g/mol]: 148.20
CAS: 1007-32-5

Physical Properties

Property code	Value	Unit	Source
gf	16.81	kJ/mol	Joback Method
hf	-125.78	kJ/mol	Joback Method
hfus	17.30	kJ/mol	Joback Method
hvap	46.88	kJ/mol	Joback Method
log10ws	-2.39		Crippen Method
logp	2.208		Crippen Method
mcvol	129.570	ml/mol	McGowan Method
pc	3142.03	kPa	Joback Method
rinpol	1192.00		NIST Webbook
rinpol	1192.00		NIST Webbook
ripol	1797.00		NIST Webbook
ripol	1797.00		NIST Webbook
tb	508.75	K	Joback Method
tc	723.65	K	Joback Method
tf	278.81	K	Joback Method
vc	0.493	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	276.61	J/mol×K	508.75	Joback Method
cpg	338.20	J/mol×K	687.83	Joback Method

cpg	327.44	J/mol×K	652.02	Joback Method
cpg	315.93	J/mol×K	616.20	Joback Method
cpg	303.65	J/mol×K	580.38	Joback Method
cpg	290.55	J/mol×K	544.57	Joback Method
cpg	348.26	J/mol×K	723.65	Joback Method
dvisc	0.0002592	Pa×s	508.75	Joback Method
dvisc	0.0003313	Pa×s	470.43	Joback Method
dvisc	0.0004422	Pa×s	432.10	Joback Method
dvisc	0.0006244	Pa×s	393.78	Joback Method
dvisc	0.0009496	Pa×s	355.46	Joback Method
dvisc	0.0015984	Pa×s	317.13	Joback Method
dvisc	0.0031046	Pa×s	278.81	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	383.70	K	2.00	NIST Webbook
tbrp	384.20	K	2.10	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=C1007325&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
rinpol:	Non-polar retention indices
ripol:	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

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