1-Pentanone, 1-(4-methylphenyl)-

Other names: 4-Methyl-1-pentanoylbenzene
4'-methylvalerophenone
Inchi: InChI=1S/C12H16O/c1-3-4-5-12(13)11-8-6-10(2)7-9-11/h6-9H,3-5H2,1-2H3
InchiKey: BCVCZJADTSTKNH-UHFFFAOYSA-N
Formula: C12H16O
SMILES: CCCCC(=O)c1ccc(C)cc1
Mol. weight [g/mol]: 176.25
CAS: 1671-77-8

Physical Properties

Property code	Value	Unit	Source
gf	24.02	kJ/mol	Joback Method
hf	-178.53	kJ/mol	Joback Method
hfus	22.09	kJ/mol	Joback Method
hvap	51.99	kJ/mol	Joback Method
ie	9.02	eV	NIST Webbook
log10ws	-3.86		Crippen Method
logp	3.368		Crippen Method
mcvol	157.750	ml/mol	McGowan Method
pc	2522.65	kPa	Joback Method
tb	559.49	K	Joback Method
tc	768.65	K	Joback Method
tf	313.87	K	Joback Method
vc	0.606	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	368.35	J/mol×K	559.49	Joback Method
cpg	383.60	J/mol×K	594.35	Joback Method
cpg	398.00	J/mol×K	629.21	Joback Method
cpg	411.56	J/mol×K	664.07	Joback Method
cpg	424.32	J/mol×K	698.93	Joback Method
cpg	436.31	J/mol×K	733.79	Joback Method

cpg	447.57	J/mol×K	768.65	Joback Method
dvisc	0.0022825	Pa×s	313.87	Joback Method
dvisc	0.0012360	Pa×s	354.81	Joback Method
dvisc	0.0007598	Pa×s	395.74	Joback Method
dvisc	0.0005117	Pa×s	436.68	Joback Method
dvisc	0.0003688	Pa×s	477.62	Joback Method
dvisc	0.0002799	Pa×s	518.55	Joback Method
dvisc	0.0002212	Pa×s	559.49	Joback Method

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=C1671778&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
ie:	Ionization energy
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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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