p-Pentylacetophenone

Other names:	p-n-Pentylacetophenone
	Acetophenone, 4'-pentyl-
	Ethanone, 1-(4-pentylphenyl)-
	4'-Pentylacetophenone
Inchi:	InChI=1S/C13H18O/c1-3-4-5-6-12-7-9-13(10-8-12)11(2)14/h7-10H,3-6H2,1-2H3
InchiKey:	KBKGPMDADJLBEM-UHFFFAOYSA-N
Formula:	C13H18O
SMILES:	CCCCCc1ccc(C(C)=O)cc1
Mol. weight [g/mol]:	190.28
CAS:	37593-02-5

Physical Properties

Property code	Value	Unit	Source
gf	32.44	kJ/mol	Joback Method
hf	-199.17	kJ/mol	Joback Method
hfus	24.68	kJ/mol	Joback Method
hvap	54.22	kJ/mol	Joback Method
log10ws	-4.19		Crippen Method
logp	3.622		Crippen Method
mcvol	171.840	ml/mol	McGowan Method
pc	2295.91	kPa	Joback Method
tb	582.37	K	Joback Method
tc	788.27	K	Joback Method
tf	325.14	K	Joback Method
vc	0.661	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	416.78	J/mol×K	582.37	Joback Method
cpg	432.70	J/mol×K	616.69	Joback Method
cpg	447.73	J/mol×K	651.00	Joback Method
cpg	461.91	J/mol×K	685.32	Joback Method
cpg	475.25	J/mol×K	719.63	Joback Method

cpg	487.80	J/mol×K	753.95	Joback Method
cpg	499.59	J/mol×K	788.27	Joback Method
dvisc	0.0022438	Pa×s	325.14	Joback Method
dvisc	0.0011931	Pa×s	368.01	Joback Method
dvisc	0.0007238	Pa×s	410.88	Joback Method
dvisc	0.0004826	Pa×s	453.75	Joback Method
dvisc	0.0003451	Pa×s	496.63	Joback Method
dvisc	0.0002603	Pa×s	539.50	Joback Method
dvisc	0.0002046	Pa×s	582.37	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	405.50 ± 0.50	K	0.50	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=C37593025&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
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