4-Acetyl-4-phenylpiperidine

Other names: Ethanone, 1-(4-phenyl-4-piperidinyl)-
methyl (4-phenyl-4-piperidyl) ketone
Inchi: InChI=1S/C13H17NO/c1-11(15)13(7-9-14-10-8-13)12-5-3-2-4-6-12/h2-6,14H,7-10H2,1H3
InchiKey: RKHWHRHOEKYEJW-UHFFFAOYSA-N
Formula: C13H17NO
SMILES: CC(=O)C1(c2ccccc2)CCNCC1
Mol. weight [g/mol]: 203.28
CAS: 34798-80-6

Physical Properties

Property code	Value	Unit	Source
gf	148.74	kJ/mol	Joback Method
hf	-80.33	kJ/mol	Joback Method
hfus	20.19	kJ/mol	Joback Method
hvap	59.59	kJ/mol	Joback Method
log10ws	-2.41		Crippen Method
logp	1.897		Crippen Method
mcvol	170.960	ml/mol	McGowan Method
pc	3096.73	kPa	Joback Method
tb	645.73	K	Joback Method
tc	902.18	K	Joback Method
tf	448.93	K	Joback Method
vc	0.629	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	451.73	J/mol×K	645.73	Joback Method
cpg	470.82	J/mol×K	688.47	Joback Method
cpg	488.63	J/mol×K	731.21	Joback Method
cpg	505.36	J/mol×K	773.95	Joback Method
cpg	521.22	J/mol×K	816.70	Joback Method
cpg	536.40	J/mol×K	859.44	Joback Method
cpg	551.12	J/mol×K	902.18	Joback Method

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=C34798806&Units=SI

Legend

cpg:	Ideal gas heat capacity
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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume