1-(6-Methyl-2-piperidyl)propan-2-one

Other names:	cis stereoisomer of 1-(6-Methyl-2-piperidyl)propan-2-one
	2-Propanone, 1-(6-methyl-2-piperidinyl)-, cis-
Inchi:	InChI=1S/C9H17NO/c1-7-4-3-5-9(10-7)6-8(2)11/h7,9-10H,3-6H2,1-2H3
InchiKey:	PLVQSRXCDPEDHN-UHFFFAOYSA-N
Formula:	C9H17NO
SMILES:	CC(=O)CC1CCCC(C)N1
Mol. weight [g/mol]:	155.24
CAS:	83285-66-9

Physical Properties

Property code	Value	Unit	Source
gf	0.43	kJ/mol	Joback Method
hf	-269.88	kJ/mol	Joback Method
hfus	23.16	kJ/mol	Joback Method
hvap	49.25	kJ/mol	Joback Method
log10ws	-2.18		Crippen Method
logp	1.496		Crippen Method
mcvol	138.360	ml/mol	McGowan Method
pc	3012.33	kPa	Joback Method
tb	522.62	K	Joback Method
tc	738.26	K	Joback Method
tf	349.29	K	Joback Method
vc	0.514	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	328.98	J/mol×K	522.62	Joback Method
cpg	346.90	J/mol×K	558.56	Joback Method
cpg	363.90	J/mol×K	594.50	Joback Method
cpg	380.01	J/mol×K	630.44	Joback Method
cpg	395.22	J/mol×K	666.38	Joback Method
cpg	409.55	J/mol×K	702.32	Joback Method
cpg	423.00	J/mol×K	738.26	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=C83285669&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
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