

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-piperidiny)-, 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

Physical Properties

Property code	Value	Unit	Source
hfus	23.16	kJ/mol	Joback Method
hvap	57.88	kJ/mol	Cheméo Relay (1.0)
ie	8.09	eV	Cheméo Relay (1.0)
log10ws	-0.54		Cheméo Relay (1.0)
logp	1.496		Crippen Method
mcvol	138.360	ml/mol	McGowan Method
tb	490.60	K	Cheméo Relay (1.0)
tf	298.18	K	Cheméo Relay (1.0)

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

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C83285669&Units=SI>

Joback Method:

https://en.wikipedia.org/wiki/Joback_method

McGowan Method:

<http://link.springer.com/article/10.1007/BF02311772>

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
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
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point

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