

2-Phenyl-1-(piperidin-1-yl)ethanone

Other names:	1-(Phenacyl)piperidine
Inchi:	InChI=1S/C13H17NO/c15-13(12-7-3-1-4-8-12)11-14-9-5-2-6-10-14/h1,3-4,7-8H,2,5-6,9-1
InchiKey:	VOIKTEMGYNKRTL-UHFFFAOYSA-N
Formula:	C13H17NO
SMILES:	O=C(CN1CCCCC1)c1ccccc1
Mol. weight [g/mol]:	203.28
CAS:	3626-62-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.69		Crippen Method
logp	2.355		Crippen Method
mcvol	170.960	ml/mol	McGowan Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hvapt	51.40	kJ/mol	413.50	NIST Webbook
hvapt	47.20	kJ/mol	416.00	NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3626628&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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