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