

1-Piperidineacetonitrile, «alpha»-phenyl-

Other names:

1-(«alpha»-Cyanobenzyl)-piperidine
«alpha»-(1-Piperidyl)-«alpha»-tolunitrile
«alpha»-Phenyl-«alpha»-(1-piperidino)-acetonitril
«alpha»-Tolunitrile-«alpha»-piperidino-
Acetonitrile, 2-phenyl-2-piperidino-
USAF A-2217
2-Phenyl-2-piperidinoacetonitrile
1-(1-Cyanobenzyl)piperidine
NSC 15446

Inchi:

InChI=1S/C13H16N2/c14-11-13(12-7-3-1-4-8-12)15-9-5-2-6-10-15/h1,3-4,7-8,13H,2,5-6,

InchiKey:

IXQJQHORYHYKBD-UHFFFAOYSA-N

Formula:

C13H16N2

SMILES:

N#CC(c1cccc1)N1CCCCC1

Mol. weight [g/mol]:

200.28

CAS:

5766-79-0

Physical Properties

Property code	Value	Unit	Source
chs	-7499.50 ± 1.20	kJ/mol	NIST Webbook
hf	190.10 ± 1.80	kJ/mol	NIST Webbook
hfs	97.20 ± 1.70	kJ/mol	NIST Webbook
hsub	73.21 ± 0.42	kJ/mol	NIST Webbook
hsub	92.90	kJ/mol	NIST Webbook
hvap	73.20 ± 0.40	kJ/mol	NIST Webbook
log10ws	-3.16		Crippen Method
logp	2.737		Crippen Method
mcvol	170.770	ml/mol	McGowan Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hfust	19.71	kJ/mol	335.20	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=C5766790&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

chs:	Standard solid enthalpy of combustion
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation at standard conditions
hfust:	Enthalpy of fusion at a given temperature
hsub:	Enthalpy of sublimation 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

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