

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(c1ccccc1)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	92.90	kJ/mol	NIST Webbook
hsub	73.21 ± 0.42	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

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
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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