

4-Benzylpiperidine

Other names:	4-(Phenylmethyl)piperidine Piperidine, 4-(phenylmethyl)- Piperidine, 4-benzyl-
Inchi:	InChI=1S/C12H17N/c1-2-4-11(5-3-1)10-12-6-8-13-9-7-12/h1-5,12-13H,6-10H2
InchiKey:	ABGXADJDTPFFSZ-UHFFFAOYSA-N
Formula:	C12H17N
SMILES:	c1ccc(CC2CCNCC2)cc1
Mol. weight [g/mol]:	175.27
CAS:	31252-42-3

Physical Properties

Property code	Value	Unit	Source
gf	274.73	kJ/mol	Joback Method
hf	37.65	kJ/mol	Joback Method
hfus	22.30	kJ/mol	Joback Method
hvap	74.20 ± 1.00	kJ/mol	NIST Webbook
log10ws	-2.79		Crippen Method
logp	2.229		Crippen Method
mcvol	155.300	ml/mol	McGowan Method
pc	3055.79	kPa	Joback Method
tb	552.20	K	NIST Webbook
tc	813.54	K	Joback Method
tf	279.50 ± 0.50	K	NIST Webbook
vc	0.570	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	381.33	J/mol×K	568.74	Joback Method
cpg	402.18	J/mol×K	609.54	Joback Method
cpg	421.58	J/mol×K	650.34	Joback Method
cpg	439.58	J/mol×K	691.14	Joback Method
cpg	456.24	J/mol×K	731.94	Joback Method
cpg	471.61	J/mol×K	772.74	Joback Method

cpg	485.75	J/mol×K	813.54	Joback Method
hvapt	72.40	kJ/mol	298.15	The vaporization enthalpy and vapor pressure of S (+)-methamphetamine at T = 298.15 K by correlation gas chromatography

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	424.20	K	2.30	NIST Webbook
tbrp	424.00 ± 1.00	K	2.30	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C31252423&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
The vaporization enthalpy and vapor pressure of S (+)-methamphetamine at 298.15 K by correlation gas chromatography:	https://www.doi.org/10.1016/j.jct.2013.08.005 https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
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
pc:	Critical Pressure

tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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