

3-Piperidinemethanol

Other names:	3-(hydroxymethyl)piperidine piperidin-3-ylmethanol
Inchi:	InChI=1S/C6H13NO/c8-5-6-2-1-3-7-4-6/h6-8H,1-5H2
InchiKey:	VUNPWIPIOOMCPT-UHFFFAOYSA-N
Formula:	C6H13NO
SMILES:	OCC1CCCNC1
Mol. weight [g/mol]:	115.17
CAS:	4606-65-9

Physical Properties

Property code	Value	Unit	Source
gf	-25.02	kJ/mol	Joback Method
hf	-227.27	kJ/mol	Joback Method
hfus	16.81	kJ/mol	Joback Method
hsub	95.90 ± 1.40	kJ/mol	NIST Webbook
hvap	52.82	kJ/mol	Joback Method
log10ws	-0.44		Crippen Method
logp	-0.022		Crippen Method
mcvol	100.390	ml/mol	McGowan Method
pc	4615.13	kPa	Joback Method
tb	496.96	K	Joback Method
tc	698.33	K	Joback Method
tf	330.61	K	Joback Method
vc	0.360	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	228.57	J/molxK	496.96	Joback Method
cpg	241.67	J/molxK	530.52	Joback Method
cpg	254.14	J/molxK	564.08	Joback Method
cpg	266.00	J/molxK	597.65	Joback Method
cpg	277.24	J/molxK	631.21	Joback Method
cpg	287.89	J/molxK	664.77	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	379.70	K	0.50	NIST Webbook

Sources

Crippen Method:https://www.chemeo.com/doc/models/crippen_log10ws**A comparative study of the volumetric properties of aqueous solutions of piperidine derivatives:**<https://www.doi.org/10.1016/j.fluid.2012.10.024>**Joback Method:**https://en.wikipedia.org/wiki/Joback_method**McGowan Method:**<http://link.springer.com/article/10.1007/BF02311772>**NIST Webbook:**<http://webbook.nist.gov/cgi/cbook.cgi?ID=C4606659&Units=SI>**Crippen Method:**<http://pubs.acs.org/doi/abs/10.1021/ci990307l>

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
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
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

<https://www.cheméo.com/cid/36-410-6/3-Piperidinemethanol.pdf>

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