

Benzenemethanol, 3-amino-

Other names:	Benzyl alcohol, m-amino- m-Aminobenzyl alcohol 3-Aminobenzyl alcohol m-Aminophenylcarbinol
Inchi:	InChI=1S/C7H9NO/c8-7-3-1-2-6(4-7)5-9/h1-4,9H,5,8H2
InchiKey:	OJZQOQNSUZLSMV-UHFFFAOYSA-N
Formula:	C7H9NO
SMILES:	<chem>Nc1cccc(CO)c1</chem>
Mol. weight [g/mol]:	123.15
CAS:	1877-77-6

Physical Properties

Property code	Value	Unit	Source
gf	40.47	kJ/mol	Joback Method
hf	-81.19	kJ/mol	Joback Method
hfus	16.82	kJ/mol	Joback Method
hvap	61.43	kJ/mol	Joback Method
log10ws	-1.25		Crippen Method
logp	0.761		Crippen Method
mcvol	101.580	ml/mol	McGowan Method
pc	4924.59	kPa	Joback Method
tb	555.93	K	Joback Method
tc	767.32	K	Joback Method
tf	351.67	K	Joback Method
vc	0.367	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	230.88	J/molxK	555.93	Joback Method
cpg	240.23	J/molxK	591.16	Joback Method
cpg	249.02	J/molxK	626.39	Joback Method
cpg	257.26	J/molxK	661.62	Joback Method
cpg	264.99	J/molxK	696.85	Joback Method

cpg	272.21	J/mol×K	732.09	Joback Method
cpg	278.97	J/mol×K	767.32	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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=C1877776&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
hvac:	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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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