2-Aminobenzyl alcohol

Other names:	Benzyl alcohol, o-amino- o-(Hydroxymethyl)aniline o-Aminobenzyl alcohol o-Aminobenzylic alcohol o-Aminophenylcarbinol Benzenemethanol, 2-amino- 2-Aminobenzenemethanol (2-Aminophenyl)methanol NSC 1173 (o-Aminophenyl)methanol
Inchi:	InChI=1S/C7H9NO/c8-7-4-2-1-3-6(7)5-9/h1-4,9H,5,8H2
InchiKey:	VYFOAVADNIHPTR-UHFFFAOYSA-N
Formula:	C7H9NO
SMILES:	Nc1ccccc1CO
Mol. weight [g/mol]:	123.15
CAS:	5344-90-1

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	548.20	K	NIST Webbook
tb	548.00 ± 5.00	K	NIST Webbook
tc	767.32	K	Joback Method
tf	357.00	K	NIST Webbook
vc	0.367	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	230.88	J/mol×K	555.93	Joback Method
cpg	240.23	J/mol×K	591.16	Joback Method
cpg	249.02	J/mol×K	626.39	Joback Method
cpg	257.26	J/mol×K	661.62	Joback Method
cpg	264.99	J/mol×K	696.85	Joback Method
cpg	272.21	J/mol×K	732.09	Joback Method
cpg	278.97	J/mol×K	767.32	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	435.20	K	2.00	NIST Webbook
tbrp	433.00	K	1.00	NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C5344901&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method: 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
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