3-(.ALPHA.-hydroxyethyl)-aniline

Other names:	(3-Aminophenyl)-1-ethanol
	m-(«alpha»-Hydroxyethyl)aniline
	3-Aminophenyl methyl carbinol
	m-Aminophenylmethylcarbinol
	m-Amino-«alpha»-methylbenzyl alcohol
	Benzenemethanol, 3-amino-«alpha»-methyl-
	m-(1-Hydroxyethyl)aniline
	Benzyl alcohol, m-amino-«alpha»-methyl-
	3-Amino-«alpha»-methylbenzyl alcohol
	1-(3-Aminophenyl)ethanol
	[3-(1-Hydroxyethyl)phenyl]amine
	NSC 62018
	NSC 8392
Inchi:	InChI=1S/C8H11NO/c1-6(10)7-3-2-4-8(9)5-7/h2-6,10H,9H2,1H3
InchiKey:	QPKNDHZQPGMLCJ-UHFFFAOYSA-N
Formula:	C8H11NO
SMILES:	CC(O)c1cccc(N)c1
Mol. weight [g/mol]:	137.18

Physical Properties

Property code	Value	Unit	Source
af	0.6496		Cheméo Relay (1.0)
hf	-159.82	kJ/mol	Cheméo Relay (1.0)
hfus	15.89	kJ/mol	Joback Method
hvap	89.10	kJ/mol	Cheméo Relay (1.0)
ie	8.14	eV	Cheméo Relay (1.0)
log10ws	-0.32		Cheméo Relay (1.0)
logp	1.322		Crippen Method
mcvol	115.670	ml/mol	McGowan Method
pc	4368.40	kPa	Joback Method
tb	529.60	K	Cheméo Relay (1.0)
tc	783.63	K	Cheméo Relay (1.0)
tf	325.36	K	Cheméo Relay (1.0)
vc	0.410	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	275.62	J/mol×K	578.37	Joback Method
cpg	286.22	J/mol×K	613.77	Joback Method
cpg	296.18	J/mol×K	649.16	Joback Method
cpg	305.51	J/mol×K	684.56	Joback Method
cpg	314.24	J/mol×K	719.95	Joback Method
cpg	322.41	J/mol×K	755.35	Joback Method
cpg	330.05	J/mol×K	790.74	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2454377&Units=SI
Joback Method: https://en.wikipedia.org/wiki/Joback_method

Legend

af: Acentric Factor
cpg: Ideal gas heat capacity
hf: Enthalpy of formation at standard conditions
hfus: Enthalpy of fusion at standard conditions
hvap: Enthalpy of vaporization at standard conditions
ie: Ionization energy
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