Benzeneethanol, 2-amino-

Other names:	2-Aminophenethyl alcohol
	Phenethyl alcohol, o-amino-
	2-(o-Aminophenyl)ethanol
	o-aminophenethyl alcohol
Inchi:	InChI=1S/C8H11NO/c9-8-4-2-1-3-7(8)5-6-10/h1-4,10H,5-6,9H2
InchiKey:	ILDXSRFKXABMHH-UHFFFAOYSA-N
Formula:	C8H11NO
SMILES:	Nc1ccccc1CCO
Mol. weight [g/mol]:	137.18
CAS:	5339-85-5

Physical Properties

Property code	Value	Unit	Source
gf	48.89	kJ/mol	Joback Method
hf	-101.83	kJ/mol	Joback Method
hfus	19.41	kJ/mol	Joback Method
hvap	63.66	kJ/mol	Joback Method
log10ws	-1.17		Crippen Method
logp	0.804		Crippen Method
mcvol	115.670	ml/mol	McGowan Method
pc	4322.57	kPa	Joback Method
tb	578.81	K	Joback Method
tc	786.81	K	Joback Method
tf	362.94	K	Joback Method
vc	0.423	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	275.18	J/mol×K	578.81	Joback Method
cpg	285.51	J/mol×K	613.48	Joback Method
cpg	295.22	J/mol×K	648.14	Joback Method
cpg	304.35	J/mol×K	682.81	Joback Method
cpg	312.92	J/mol×K	717.48	Joback Method

cpg	320.95	J/mol×K	752.15	Joback Method
cpg	328.47	J/mol×K	786.81	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	420.70	K	0.50	NIST Webbook
tbrp	428.00	K	0.70	NIST Webbook
tbrp	420.50 ± 0.50	K	0.47	NIST Webbook

Sources

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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C5339855&Units=SI

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