

4-(1-Aminoethyl)phenol

Inchi:	InChI=1S/C8H11NO/c1-6(9)7-2-4-8(10)5-3-7/h2-6,10H,9H2,1H3
InchiKey:	CDQPLIAKRDYOCB-UHFFFAOYSA-N
Formula:	C8H11NO
SMILES:	CC(N)c1ccc(O)cc1
Mol. weight [g/mol]:	137.18
CAS:	134855-87-1

Physical Properties

Property code	Value	Unit	Source
gf	38.28	kJ/mol	Joback Method
hf	-120.72	kJ/mol	Joback Method
hfus	17.97	kJ/mol	Joback Method
hvap	58.95	kJ/mol	Joback Method
log10ws	-1.72		Crippen Method
logp	1.412		Crippen Method
mcvol	115.670	ml/mol	McGowan Method
pc	4815.84	kPa	Joback Method
tb	561.83	K	Joback Method
tc	803.03	K	Joback Method
tf	386.32	K	Joback Method
vc	0.364	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	276.91	J/molxK	561.83	Joback Method
cpg	288.84	J/molxK	602.03	Joback Method
cpg	299.84	J/molxK	642.23	Joback Method
cpg	310.01	J/molxK	682.43	Joback Method
cpg	319.44	J/molxK	722.63	Joback Method
cpg	328.23	J/molxK	762.83	Joback Method
cpg	336.49	J/molxK	803.03	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C134855871&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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

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
mccvol:	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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