Phenol, 4-(2-aminoethyl)-2-methoxy-

Other names:	3-Methoxy-4-hydroxyphenylethyl amine
	4-(2-aminoethyl)-2-methoxy-phenol
	Methoxy phenolethylamin
Inchi:	InChI=1S/C9H13NO2/c1-12-9-6-7(4-5-10)2-3-8(9)11/h2-3,6,11H,4-5,10H2,1H3
InchiKey:	DIVQKHQLANKJQO-UHFFFAOYSA-N
Formula:	C9H13NO2
SMILES:	COc1cc(CCN)ccc1O
Mol. weight [g/mol]:	167.21
CAS:	554-52-9

Physical Properties

Property code	Value	Unit	Source
gf	-65.49	kJ/mol	Joback Method
hf	-279.77	kJ/mol	Joback Method
hfus	24.89	kJ/mol	Joback Method
hvap	64.63	kJ/mol	Joback Method
log10ws	-1.38		Crippen Method
logp	0.902		Crippen Method
mcvol	135.630	ml/mol	McGowan Method
pc	4021.02	kPa	Joback Method
tb	612.55	K	Joback Method
tc	841.41	K	Joback Method
tf	447.34	K	Joback Method
vc	0.445	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	343.92	J/mol×K	612.55	Joback Method
cpg	355.92	J/mol×K	650.69	Joback Method
cpg	367.17	J/mol×K	688.84	Joback Method
cpg	377.74	J/mol×K	726.98	Joback Method
cpg	387.69	J/mol×K	765.12	Joback Method
cpg	397.08	J/mol×K	803.27	Joback Method

cpg	405.97	J/mol×K	841.41	Joback Method

Sources

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=C554529&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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