4-(2-AMINOETHYL)-2-METHOXYPHENOL

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

Physical Properties

Property code	Value	Unit	Source
hf	-256.91	kJ/mol	Cheméo Relay (1.0)
hfus	24.89	kJ/mol	Joback Method
hvap	79.63	kJ/mol	Cheméo Relay (1.0)
ie	8.03	eV	Cheméo Relay (1.0)
log10ws	-1.06		Cheméo Relay (1.0)
logp	0.902		Crippen Method
mcvol	135.630	ml/mol	McGowan Method
tb	562.09	K	Cheméo Relay (1.0)
tf	410.72	K	Cheméo Relay (1.0)

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

Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C554529&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
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):	

Legend

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
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point