

5-Amino-2-methoxyphenol, N,N-methyl-, methyl ether

Inchi:	InChI=1S/C10H15NO2/c1-11(2)8-5-6-9(12-3)10(7-8)13-4/h5-7H,1-4H3
InchiKey:	OJSINGAPXRDNSN-UHFFFAOYSA-N
Formula:	C10H15NO2
SMILES:	COc1ccc(N(C)C)cc1OC
Mol. weight [g/mol]:	181.23

Physical Properties

Property code	Value	Unit	Source
gf	27.25	kJ/mol	Joback Method
hf	-233.05	kJ/mol	Joback Method
hfus	20.32	kJ/mol	Joback Method
hvap	48.32	kJ/mol	Joback Method
log10ws	-1.62		Crippen Method
logp	1.770		Crippen Method
mcvol	149.720	ml/mol	McGowan Method
pc	2732.56	kPa	Joback Method
rinsol	1536.70		NIST Webbook
tb	522.12	K	Joback Method
tc	723.28	K	Joback Method
tf	330.85	K	Joback Method
vc	0.541	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	339.87	J/mol×K	522.12	Joback Method
cpg	354.34	J/mol×K	555.65	Joback Method
cpg	368.15	J/mol×K	589.17	Joback Method
cpg	381.32	J/mol×K	622.70	Joback Method
cpg	393.85	J/mol×K	656.22	Joback Method
cpg	405.73	J/mol×K	689.75	Joback Method
cpg	416.97	J/mol×K	723.28	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U352886&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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