3-Dimethylaminoanisole

Other names: 3-Methoxy-N,N-dimethylaniline
3-Methoxy-N,N-dimethylbenzenamine
Inchi: InChI=1S/C9H13NO/c1-10(2)8-5-4-6-9(7-8)11-3/h4-7H,1-3H3
InchiKey: MOYHVSKDHLMMPS-UHFFFAOYSA-N
Formula: C9H13NO
SMILES: COc1cccc(N(C)C)c1
Mol. weight [g/mol]: 151.21
CAS: 15799-79-8

Physical Properties

Property code	Value	Unit	Source
affp	920.60	kJ/mol	NIST Webbook
basg	894.10	kJ/mol	NIST Webbook
gf	133.46	kJ/mol	Joback Method
hf	-68.72	kJ/mol	Joback Method
hfus	16.93	kJ/mol	Joback Method
hvap	43.02	kJ/mol	Joback Method
log10ws	-1.50		Crippen Method
logp	1.761		Crippen Method
mcvol	129.760	ml/mol	McGowan Method
pc	3138.51	kPa	Joback Method
tb	471.84	K	Joback Method
tc	676.27	K	Joback Method
tf	284.83	K	Joback Method
vc	0.468	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	270.72	J/mol×K	471.84	Joback Method
cpg	284.89	J/mol×K	505.91	Joback Method
cpg	298.34	J/mol×K	539.98	Joback Method
cpg	311.09	J/mol×K	574.05	Joback Method
cpg	323.14	J/mol×K	608.12	Joback Method

cpg	334.54	J/mol×K	642.20	Joback Method
cpg	345.28	J/mol×K	676.27	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C15799798&Units=SI
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

Legend

affp:	Proton affinity
basg:	Gas basicity
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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