p-Methoxybenzamide

Other names:	4-methoxybenzamide
	Benzamide, 4-methoxy-
	p-anisamide
Inchi:	InChI=1S/C8H9NO2/c1-11-7-4-2-6(3-5-7)8(9)10/h2-5H,1H3,(H2,9,10)
InchiKey:	GUCPYIYFQVTFSI-UHFFFAOYSA-N
Formula:	C8H9NO2
SMILES:	COc1ccc(C(N)=O)cc1
Mol. weight [g/mol]:	151.16
CAS:	3424-93-9

Physical Properties

Property code	Value	Unit	Source
affp	900.30	kJ/mol	NIST Webbook
basg	869.40	kJ/mol	NIST Webbook
gf	-48.21	kJ/mol	Joback Method
hf	-194.40	kJ/mol	Joback Method
hfus	29.04	kJ/mol	The thermodynamic stability of the three isomers of methoxybenzamide: An experimental and computational study
hvap	56.14	kJ/mol	Joback Method
ie	8.62	eV	NIST Webbook
log10ws	-1.76		Crippen Method
logp	0.794		Crippen Method
mcvol	117.240	ml/mol	McGowan Method
pc	4072.51	kPa	Joback Method
rinpol	1626.70		NIST Webbook
rinpol	1626.70		NIST Webbook
tb	568.20	K	NIST Webbook
tc	793.64	K	Joback Method
tf	374.28	K	Joback Method
vc	0.428	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	264.93	J/mol×K	562.92	Joback Method
cpg	276.15	J/mol×K	601.37	Joback Method
cpg	286.68	J/mol×K	639.83	Joback Method
cpg	296.53	J/mol×K	678.28	Joback Method
cpg	305.72	J/mol×K	716.73	Joback Method
cpg	314.25	J/mol×K	755.19	Joback Method
cpg	322.15	J/mol×K	793.64	Joback Method

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

The thermodynamic stability of the three isomers of methoxybenzamide: An experimental and computational study: https://www.doi.org/10.1016/j.jct.2013.06.022

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=C3424939&Units=SI

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

ie: Ionization energy

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

pc: Critical Pressure

rinpol: Non-polar retention indices

tb: Normal Boiling Point Temperature

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