Benzoic acid, 4-(methylamino)-

Other names:	Benzoic acid, p-(methylamino)-
	p-(Methylamino)benzoic acid
	N-Methyl-4-aminobenzoic acid
	4-(Methylamino)benzoic acid
	4-(N-Methylamino)benzoic acid
	p-(N-Methylamino)benzoic acid
Inchi:	InChI=1S/C8H9NO2/c1-9-7-4-2-6(3-5-7)8(10)11/h2-5,9H,1H3,(H,10,11)
InchiKey:	ZVIDMSBTYRSMAR-UHFFFAOYSA-N
Formula:	C8H9NO2
SMILES:	CNc1ccc(C(=O)O)cc1
Mol. weight [g/mol]:	151.16
CAS:	10541-83-0

Physical Properties

Property code	Value	Unit	Source
gf	-57.09	kJ/mol	Joback Method
hf	-194.73	kJ/mol	Joback Method
hfus	20.91	kJ/mol	Joback Method
hvap	66.20	kJ/mol	Joback Method
ie	8.10	eV	NIST Webbook
ie	7.30	eV	NIST Webbook
log10ws	-1.54		Crippen Method
logp	1.426		Crippen Method
mcvol	117.240	ml/mol	McGowan Method
pc	4432.62	kPa	Joback Method
tb	610.32	K	Joback Method
tc	817.72	K	Joback Method
tf	382.27	K	Joback Method
vc	0.435	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	278.76	J/mol×K	610.32	Joback Method

cpg	288.23	J/mol×K	644.89	Joback Method
cpg	297.10	J/mol×K	679.45	Joback Method
cpg	305.39	J/mol×K	714.02	Joback Method
cpg	313.13	J/mol×K	748.59	Joback Method
cpg	320.34	J/mol×K	783.15	Joback Method
cpg	327.05	J/mol×K	817.72	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C10541830&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
ie:	Ionization energy
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