Benzoic acid, 4-(dimethylamino)-

Other names:	Benzoic acid, p-(dimethylamino)-
	p-(Dimethylamino)benzoic acid
	p-N,N-(Dimethylamino)benzoic acid
	N,N-Dimethyl-4-aminobenzoic acid
	4-(Dimethylamino)benzoic acid
	N,N-Dimethyl-p-aminobenzoic acid
	NSC 16596
Inchi:	InChI=1S/C9H11NO2/c1-10(2)8-5-3-7(4-6-8)9(11)12/h3-6H,1-2H3,(H,11,12)
InchiKey:	YDIYEOMDOWUDTJ-UHFFFAOYSA-N
Formula:	C9H11NO2
SMILES:	CN(C)c1ccc(C(=O)O)cc1
Mol. weight [g/mol]:	165.19
CAS:	619-84-1

Physical Properties

Property code	Value	Unit	Source
gf	-27.28	kJ/mol	Joback Method
hf	-201.31	kJ/mol	Joback Method
hfus	21.43	kJ/mol	Joback Method
hvap	64.03	kJ/mol	Joback Method
ie	7.10	eV	NIST Webbook
ie	7.80	eV	NIST Webbook
log10ws	-1.44		Crippen Method
logp	1.451		Crippen Method
mcvol	131.330	ml/mol	McGowan Method
pc	3843.54	kPa	Joback Method
tb	595.47	K	Joback Method
tc	796.97	K	Joback Method
tf	373.35	K	Joback Method
vc	0.474	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	315.31	J/mol×K	595.47	Joback Method
cpg	326.16	J/mol×K	629.05	Joback Method
cpg	336.34	J/mol×K	662.64	Joback Method
cpg	345.87	J/mol×K	696.22	Joback Method
cpg	354.78	J/mol×K	729.81	Joback Method
cpg	363.11	J/mol×K	763.39	Joback Method
cpg	370.88	J/mol×K	796.97	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C619841&Units=SI

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