Benzoic acid, 2-(methylamino)-

Other names:	2-(Methylamino)benzoic acid
	Anthranilic acid, N-methyl-
	Kyselina 2-methylaminobenzoova
	Kyselina N-methylanthranilova
	N-Methyl-2-aminobenzoic acid
	N-Methyl-o-aminobenzoic acid
	N-Methylanthranilic acid
	o-(Methylamino)benzoic acid
Inchi:	InChI=1S/C8H9NO2/c1-9-7-5-3-2-4-6(7)8(10)11/h2-5,9H,1H3,(H,10,11)
InchiKey:	WVMBPWMAQDVZCM-UHFFFAOYSA-N
Formula:	C8H9NO2
SMILES:	CNc1ccccc1C(=O)O
Mol. weight [g/mol]:	151.16
CAS:	119-68-6

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
log10ws	-2.88		Aqueous Solubility Prediction 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	453.65	K	Aqueous Solubility Prediction 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

Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C119686&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Joback Method: https://en.wikipedia.org/wiki/Joback_method

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