Benzoic acid, 2(methylamino)methyl

Inchi: InChI=1S/C9H11NO2/c1-10-6-7-4-2-3-5-8(7)9(11)12/h2-5,10H,6H2,1H3,(H,11,12)
InchiKey: OEPGNWSDEDOQHX-UHFFFAOYSA-N
Formula: C9H11NO2
SMILES: CNCc1ccccc1C(=O)O
Mol. weight [g/mol]: 165.19

Physical Properties

Property code	Value	Unit	Source
gf	-48.67	kJ/mol	Joback Method
hf	-215.37	kJ/mol	Joback Method
hfus	23.50	kJ/mol	Joback Method
hvap	68.43	kJ/mol	Joback Method
log10ws	-2.02		Crippen Method
logp	1.104		Crippen Method
mcvol	131.330	ml/mol	McGowan Method
pc	3916.03	kPa	Joback Method
rinpol	1484.00		NIST Webbook
tb	633.20	K	Joback Method
tc	837.52	K	Joback Method
tf	393.54	K	Joback Method
vc	0.491	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	325.55	J/mol×K	633.20	Joback Method
cpg	335.83	J/mol×K	667.25	Joback Method
cpg	345.47	J/mol×K	701.31	Joback Method
cpg	354.50	J/mol×K	735.36	Joback Method
cpg	362.94	J/mol×K	769.41	Joback Method
cpg	370.82	J/mol×K	803.46	Joback Method
cpg	378.17	J/mol×K	837.52	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R576484&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

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume