2-Dimethylaminobenzoic acid

Other names: Benzoic acid, 2-(dimethylamino)-
Anthranilic acid, N,N-dimethyl-
N,N-Dimethylanthranilic acid
Inchi: InChI=1S/C9H11NO2/c1-10(2)8-6-4-3-5-7(8)9(11)12/h3-6H,1-2H3,(H,11,12)
InchiKey: DVVXXHVHGGWWPE-UHFFFAOYSA-N
Formula: C9H11NO2
SMILES: CN(C)c1ccccc1C(=O)O
Mol. weight [g/mol]: 165.19
CAS: 610-16-2

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
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=C610162&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
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