anthranilic acid

Other names: 2-aminobenzoic acid
Inchi: InChI=1S/C7H7NO2/c8-6-4-2-1-3-5(6)7(9)10/h1-4H,8H2,(H,9,10)
InchiKey: RWZYAGGXGHYGMB-UHFFFAOYSA-N
Formula: C7H7NO2
SMILES: Nc1ccccc1C(=O)O
Mol. weight [g/mol]: 137.14
CAS: 118-92-3

Physical Properties

Property code	Value	Unit	Source
affp	901.50	kJ/mol	NIST Webbook
basg	869.00	kJ/mol	NIST Webbook
chs	-3354.00 ± 0.80	kJ/mol	NIST Webbook
chs	-3353.83 ± 0.80	kJ/mol	NIST Webbook
gf	-88.45	kJ/mol	Joback Method
hf	-296.20 ± 1.60	kJ/mol	NIST Webbook
hfs	-401.00 ± 0.80	kJ/mol	NIST Webbook
hfs	-401.10 ± 1.20	kJ/mol	NIST Webbook
hfus	18.42	kJ/mol	Joback Method
hsub	111.60 ± 1.70	kJ/mol	NIST Webbook
hsub	104.90 ± 1.00	kJ/mol	NIST Webbook
hsub	104.90 ± 1.00	kJ/mol	NIST Webbook
hvap	68.18	kJ/mol	Joback Method
ie	7.60	eV	NIST Webbook
ie	8.29	eV	NIST Webbook
ie	8.00	eV	NIST Webbook
log10ws	-1.52		Aqueous Solubility Prediction Method
logp	0.967		Crippen Method
mcvol	103.150	ml/mol	McGowan Method
pc	5390.71	kPa	Joback Method
rinpol	1413.10		NIST Webbook
rinpol	1416.00		NIST Webbook
rinpol	1413.10		NIST Webbook
ripol	3021.00		NIST Webbook
ripol	2997.00		NIST Webbook
tb	609.80	K	Joback Method

tc	828.81	K	Joback Method
tf	417.80 ± 0.50	K	NIST Webbook
vc	0.373	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	240.14	J/mol×K	609.80	Joback Method
cpg	275.91	J/mol×K	792.31	Joback Method
cpg	269.79	J/mol×K	755.81	Joback Method
cpg	263.18	J/mol×K	719.31	Joback Method
cpg	256.05	J/mol×K	682.80	Joback Method
cpg	248.38	J/mol×K	646.30	Joback Method
cpg	281.56	J/mol×K	828.81	Joback Method
cps	165.30	J/mol×K	298.00	NIST Webbook
cps	187.00	J/mol×K	323.00	NIST Webbook
hfust	20.38	kJ/mol	417.80	NIST Webbook
hfust	20.50	kJ/mol	417.80	NIST Webbook
hfust	20.50	kJ/mol	417.80	NIST Webbook
sfust	48.80	J/mol×K	417.80	NIST Webbook

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method
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=C118923&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

affp: Proton affinity
basg: Gas basicity
chs: Standard solid enthalpy of combustion
cpg: Ideal gas heat capacity
cps: Solid phase heat capacity

gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
hsub:	Enthalpy of sublimation 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
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
sfust:	Entropy of fusion at a given temperature
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume