3-Aminosalicylic acid

Other names: Benzoic acid, 3-amino-2-hydroxy-
Salicylic acid, 3-amino-
Inchi: InChI=1S/C7H7NO3/c8-5-3-1-2-4(6(5)9)7(10)11/h1-3,9H,8H2,(H,10,11)
InchiKey: IQGMRVWUTCYCST-UHFFFAOYSA-N
Formula: C7H7NO3
SMILES: Nc1cccc(C(=O)O)c1O
Mol. weight [g/mol]: 153.14
CAS: 570-23-0

Physical Properties

Property code	Value	Unit	Source
gf	-243.07	kJ/mol	Joback Method
hf	-371.08	kJ/mol	Joback Method
hfus	24.21	kJ/mol	Joback Method
hvap	81.19	kJ/mol	Joback Method
log10ws	-0.71		Crippen Method
logp	0.673		Crippen Method
mcvol	109.020	ml/mol	McGowan Method
pc	6796.39	kPa	Joback Method
tb	690.42	K	Joback Method
tc	918.13	K	Joback Method
tf	513.32	K	Joback Method
vc	0.340	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	277.00	J/mol×K	690.42	Joback Method
cpg	283.98	J/mol×K	728.37	Joback Method
cpg	290.51	J/mol×K	766.32	Joback Method
cpg	296.65	J/mol×K	804.27	Joback Method
cpg	302.48	J/mol×K	842.23	Joback Method
cpg	308.08	J/mol×K	880.18	Joback Method
cpg	313.51	J/mol×K	918.13	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C570230&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume