Benzenesulfonic acid, 5-amino-2-hydroxy-

Other names: 5-amino-2-hydroxybenzenesulphonic acid
Inchi: InChI=1S/C6H7NO4S/c7-4-1-2-5(8)6(3-4)12(9,10)11/h1-3,8H,7H2,(H,9,10,11)
InchiKey: SILINKWDNDDXTL-UHFFFAOYSA-N
Formula: C6H7NO4S
SMILES: Nc1ccc(O)c(S(=O)(=O)O)c1
Mol. weight [g/mol]: 189.19
CAS: 2835-04-3

Physical Properties

Property code	Value	Unit	Source
gf	-591.11	kJ/mol	Joback Method
hf	-691.21	kJ/mol	Joback Method
hfus	31.39	kJ/mol	Joback Method
hvap	90.86	kJ/mol	Joback Method
log10ws	-0.24		Crippen Method
logp	0.221		Crippen Method
mcvol	121.450	ml/mol	McGowan Method
pc	9518.14	kPa	Joback Method
tb	661.45	K	Joback Method
tc	878.13	K	Joback Method
tf	490.68	K	Joback Method
vc	0.404	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	301.22	J/mol×K	661.45	Joback Method
cpg	308.71	J/mol×K	697.56	Joback Method
cpg	315.63	J/mol×K	733.68	Joback Method
cpg	322.05	J/mol×K	769.79	Joback Method
cpg	327.99	J/mol×K	805.90	Joback Method
cpg	333.49	J/mol×K	842.01	Joback Method
cpg	338.61	J/mol×K	878.13	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2835043&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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