Benzenesulfonic acid, 2-amino-5-chloro-4-ethyl-

Other names: 2-Amino-5-chloro-4-ethylbenzenesulfonic acid
2-amino-5-chloro-4-ethylbenzenesulphonic acid
Inchi: InChI=1S/C8H10ClNO3S/c1-2-5-3-7(10)8(4-6(5)9)14(11,12)13/h3-4H,2,10H2,1H3,(H,11,
InchiKey: DJOIZOKQHNHZPN-UHFFFAOYSA-N
Formula: C8H10ClNO3S
SMILES: CCc1cc(N)c(S(=O)(=O)O)cc1Cl
Mol. weight [g/mol]: 235.69
CAS: 88-56-2

Physical Properties

Property code	Value	Unit	Source
gf	-450.84	kJ/mol	Joback Method
hf	-593.86	kJ/mol	Joback Method
hfus	34.21	kJ/mol	Joback Method
hvap	88.00	kJ/mol	Joback Method
log10ws	-2.18		Crippen Method
logp	1.731		Crippen Method
mcvol	156.000	ml/mol	McGowan Method
pc	4869.76	kPa	Joback Method
tb	673.98	K	Joback Method
tc	880.44	K	Joback Method
tf	456.46	K	Joback Method
vc	0.599	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	373.44	J/mol×K	673.98	Joback Method
cpg	382.78	J/mol×K	708.39	Joback Method
cpg	391.48	J/mol×K	742.80	Joback Method
cpg	399.56	J/mol×K	777.21	Joback Method
cpg	407.00	J/mol×K	811.62	Joback Method
cpg	413.81	J/mol×K	846.03	Joback Method
cpg	419.98	J/mol×K	880.44	Joback Method

Sources

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=C88562&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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