4-Amino-2-chloro-5(methylsulfamyl)benzenesulfo

Inchi: InChI=1S/C7H10ClN3O4S2/c1-11-17(14,15)7-3-6(16(10,12)13)4(8)2-5(7)9/h2-3,11H,9H2
InchiKey: HZLMCYKKQJTLER-UHFFFAOYSA-N
Formula: C7H10ClN3O4S2
SMILES: CNS(=O)(=O)c1cc(S(N)(=O)=O)c(Cl)cc1N
Mol. weight [g/mol]: 299.75
CAS: 13659-98-8

Physical Properties

Property code	Value	Unit	Source
gf	-635.14	kJ/mol	Joback Method
hf	-787.08	kJ/mol	Joback Method
hfus	49.21	kJ/mol	Joback Method
hvap	104.81	kJ/mol	Joback Method
log10ws	-1.36		Crippen Method
logp	-0.522		Crippen Method
mcvol	184.090	ml/mol	McGowan Method
pc	6898.38	kPa	Joback Method
tb	729.40	K	Joback Method
tc	952.11	K	Joback Method
tf	558.85	K	Joback Method
vc	0.714	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	459.91	J/mol×K	729.40	Joback Method
cpg	469.74	J/mol×K	766.52	Joback Method
cpg	478.58	J/mol×K	803.64	Joback Method
cpg	486.44	J/mol×K	840.75	Joback Method
cpg	493.27	J/mol×K	877.87	Joback Method
cpg	499.08	J/mol×K	914.99	Joback Method
cpg	503.83	J/mol×K	952.11	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C13659988&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