4-Amino-6-methyl-1,3-benzenedisulfonamide

Inchi: InChI=1S/C7H11N3O4S2/c1-4-2-5(8)7(16(10,13)14)3-6(4)15(9,11)12/h2-3H,8H2,1H3,(H
InchiKey: JGFQDYAUPNZBMU-UHFFFAOYSA-N
Formula: C7H11N3O4S2
SMILES: Cc1cc(N)c(S(N)(=O)=O)cc1S(N)(=O)=O
Mol. weight [g/mol]: 265.31
CAS: 1020-33-3

Physical Properties

Property code	Value	Unit	Source
gf	-646.15	kJ/mol	Joback Method
hf	-791.02	kJ/mol	Joback Method
hfus	45.11	kJ/mol	Joback Method
hvap	104.63	kJ/mol	Joback Method
log10ws	-0.98		Crippen Method
logp	-1.128		Crippen Method
mcvol	171.850	ml/mol	McGowan Method
pc	7929.40	kPa	Joback Method
tb	714.33	K	Joback Method
tc	941.43	K	Joback Method
tf	559.53	K	Joback Method
vc	0.658	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	445.35	J/mol×K	714.33	Joback Method
cpg	455.86	J/mol×K	752.18	Joback Method
cpg	465.38	J/mol×K	790.03	Joback Method
cpg	473.89	J/mol×K	827.88	Joback Method
cpg	481.37	J/mol×K	865.73	Joback Method
cpg	487.78	J/mol×K	903.58	Joback Method
cpg	493.12	J/mol×K	941.43	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1020333&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