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

Inchi: InChI=1S/C6H8BrN3O4S2/c7-3-1-4(8)6(16(10,13)14)2-5(3)15(9,11)12/h1-2H,8H2,(H2,9,
InchiKey: YRXAPDMJILMLSU-UHFFFAOYSA-N
Formula: C6H8BrN3O4S2
SMILES: Nc1cc(Br)c(S(N)(=O)=O)cc1S(N)(=O)=O
Mol. weight [g/mol]: 330.18
CAS: 1020-32-2

Physical Properties

Property code	Value	Unit	Source
gf	-640.25	kJ/mol	Joback Method
hf	-744.05	kJ/mol	Joback Method
hfus	47.80	kJ/mol	Joback Method
hvap	108.84	kJ/mol	Joback Method
log10ws	-1.67		Crippen Method
logp	-0.674		Crippen Method
mcvol	175.260	ml/mol	McGowan Method
pc	10896.05	kPa	Joback Method
tb	757.61	K	Joback Method
tc	998.97	K	Joback Method
tf	608.06	K	Joback Method
vc	0.664	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	423.24	J/mol×K	757.61	Joback Method
cpg	431.44	J/mol×K	797.84	Joback Method
cpg	438.61	J/mol×K	838.06	Joback Method
cpg	444.74	J/mol×K	878.29	Joback Method
cpg	449.79	J/mol×K	918.52	Joback Method
cpg	453.75	J/mol×K	958.75	Joback Method
cpg	456.61	J/mol×K	998.97	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1020322&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