m-Aminobenzenesulfonyl fluoride

Other names:	Benzenesulfonyl fluoride, 3-amino-
	Metanilyl fluoride
Inchi:	InChI=1S/C6H6FNO2S/c7-11(9,10)6-3-1-2-5(8)4-6/h1-4H,8H2
InchiKey:	PLSYVJDMJWGODG-UHFFFAOYSA-N
Formula:	C6H6FNO2S
SMILES:	Nc1cccc(S(=O)(=O)F)c1
Mol. weight [g/mol]:	175.18
CAS:	368-50-3

Physical Properties

Property code	Value	Unit	Source
gf	-494.48	kJ/mol	Joback Method
hf	-557.78	kJ/mol	Joback Method
hfus	24.60	kJ/mol	Joback Method
hvap	60.35	kJ/mol	Joback Method
log10ws	-1.22		Crippen Method
logp	0.927		Crippen Method
mcvol	111.480	ml/mol	McGowan Method
pc	5818.28	kPa	Joback Method
tb	487.92	K	Joback Method
tc	699.38	K	Joback Method
tf	318.73	K	Joback Method
vc	0.436	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	227.96	J/mol×K	487.92	Joback Method
cpg	238.17	J/mol×K	523.16	Joback Method
cpg	247.79	J/mol×K	558.41	Joback Method
cpg	256.82	J/mol×K	593.65	Joback Method
cpg	265.27	J/mol×K	628.90	Joback Method
cpg	273.13	J/mol×K	664.14	Joback Method
cpg	280.41	J/mol×K	699.38	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C368503&Units=SI

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