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

Physical Properties

Property code	Value	Unit	Source
af	0.5511		Cheméo Relay (1.0)
hfus	24.60	kJ/mol	Joback Method
hvap	82.82	kJ/mol	Cheméo Relay (1.0)
ie	8.69	eV	Cheméo Relay (1.0)
log10ws	-1.91		Cheméo Relay (1.0)
logp	0.927		Crippen Method
mcvol	111.480	ml/mol	McGowan Method
pc	5818.28	kPa	Joback Method
tb	556.03	K	Cheméo Relay (1.0)
tc	801.33	K	Cheméo Relay (1.0)
tf	388.36	K	Cheméo Relay (1.0)

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

Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C368503&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

af:	Acentric Factor
cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
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