3-Amino-4-chlorobenzenesulfonyl fluoride

Other names: Benzenesulfonyl fluoride, 3-amino-4-chloro-
3-amino-4-chlorobenzenesulphonyl fluoride
Inchi: InChI=1S/C6H5ClFNO2S/c7-5-2-1-4(3-6(5)9)12(8,10)11/h1-3H,9H2
InchiKey: HNZYBSQZUOJCDN-UHFFFAOYSA-N
Formula: C6H5ClFNO2S
SMILES: Nc1cc(S(=O)(=O)F)ccc1Cl
Mol. weight [g/mol]: 209.63
CAS: 368-72-9

Physical Properties

Property code	Value	Unit	Source
gf	-516.04	kJ/mol	Joback Method
hf	-584.99	kJ/mol	Joback Method
hfus	28.41	kJ/mol	Joback Method
hvap	65.39	kJ/mol	Joback Method
log10ws	-1.91		Crippen Method
logp	1.580		Crippen Method
mcvol	123.720	ml/mol	McGowan Method
pc	5382.80	kPa	Joback Method
tb	530.33	K	Joback Method
tc	748.18	K	Joback Method
tf	361.17	K	Joback Method
vc	0.485	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	250.17	J/mol×K	530.33	Joback Method
cpg	259.36	J/mol×K	566.64	Joback Method
cpg	267.99	J/mol×K	602.95	Joback Method
cpg	276.04	J/mol×K	639.25	Joback Method
cpg	283.52	J/mol×K	675.56	Joback Method
cpg	290.43	J/mol×K	711.87	Joback Method
cpg	296.76	J/mol×K	748.18	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C368729&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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