3-Amino-4-(methylthio)benzotrifluoride

Inchi: InChI=1S/C8H8F3NS/c1-13-7-3-2-5(4-6(7)12)8(9,10)11/h2-4H,12H2,1H3
InchiKey: OQFOLJGOVFYDHZ-UHFFFAOYSA-N
Formula: C8H8F3NS
SMILES: CSc1ccc(C(F)(F)F)cc1N
Mol. weight [g/mol]: 207.22
CAS: 207974-07-0

Physical Properties

Property code	Value	Unit	Source
gf	-372.39	kJ/mol	Joback Method
hf	-516.28	kJ/mol	Joback Method
hfus	20.89	kJ/mol	Joback Method
hvap	50.71	kJ/mol	Joback Method
log10ws	-2.95		Crippen Method
logp	3.010		Crippen Method
mcvol	131.460	ml/mol	McGowan Method
pc	3352.86	kPa	Joback Method
tb	554.97	K	Joback Method
tc	780.14	K	Joback Method
tf	353.23	K	Joback Method
vc	0.501	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	303.42	J/mol×K	554.97	Joback Method
cpg	314.77	J/mol×K	592.50	Joback Method
cpg	325.27	J/mol×K	630.03	Joback Method
cpg	334.98	J/mol×K	667.55	Joback Method
cpg	343.93	J/mol×K	705.08	Joback Method
cpg	352.16	J/mol×K	742.61	Joback Method
cpg	359.73	J/mol×K	780.14	Joback Method

Sources

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=C207974070&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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