2-Amino-3-fluorobenzotrifluoride

Inchi: InChI=1S/C7H5F4N/c8-5-3-1-2-4(6(5)12)7(9,10)11/h1-3H,12H2
InchiKey: CQSFHEFEKDRLKE-UHFFFAOYSA-N
Formula: C7H5F4N
SMILES: Nc1c(F)cccc1C(F)(F)F
Mol. weight [g/mol]: 179.11
CAS: 144851-61-6

Physical Properties

Property code	Value	Unit	Source
gf	-608.74	kJ/mol	Joback Method
hf	-733.62	kJ/mol	Joback Method
hfus	17.25	kJ/mol	Joback Method
hvap	40.85	kJ/mol	Joback Method
log10ws	-2.54		Crippen Method
logp	2.427		Crippen Method
mcvol	102.790	ml/mol	McGowan Method
pc	3488.88	kPa	Joback Method
tb	462.58	K	Joback Method
tc	659.44	K	Joback Method
tf	308.15	K	Joback Method
vc	0.409	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	224.78	J/mol×K	462.58	Joback Method
cpg	234.58	J/mol×K	495.39	Joback Method
cpg	243.72	J/mol×K	528.20	Joback Method
cpg	252.24	J/mol×K	561.01	Joback Method
cpg	260.15	J/mol×K	593.82	Joback Method
cpg	267.50	J/mol×K	626.63	Joback Method
cpg	274.32	J/mol×K	659.44	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=C144851616&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