

3-Amino-2-fluorobenzotrifluoride

Inchi:	InChI=1S/C7H5F4N/c8-6-4(7(9,10)11)2-1-3-5(6)12/h1-3H,12H2
InchiKey:	YKPDYPPZLUZONK-UHFFFAOYSA-N
Formula:	C7H5F4N
SMILES:	Nc1cccc(C(F)(F)F)c1F
Mol. weight [g/mol]:	179.11
CAS:	123973-25-1

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/molxK	462.58	Joback Method
cpg	234.58	J/molxK	495.39	Joback Method
cpg	243.72	J/molxK	528.20	Joback Method
cpg	252.24	J/molxK	561.01	Joback Method
cpg	260.15	J/molxK	593.82	Joback Method
cpg	267.50	J/molxK	626.63	Joback Method
cpg	274.32	J/molxK	659.44	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C123973251&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
mccvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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