2-Amino-6-fluorobenzonitrile

Other names: Benzonitrile, 2-amino-6-fluoro-
Inchi: InChI=1S/C7H5FN2/c8-6-2-1-3-7(10)5(6)4-9/h1-3H,10H2
InchiKey: IQUNZGOZUJITBJ-UHFFFAOYSA-N
Formula: C7H5FN2
SMILES: N#Cc1c(N)cccc1F
Mol. weight [g/mol]: 136.13
CAS: 77326-36-4

Physical Properties

Property code	Value	Unit	Source
gf	106.03	kJ/mol	Joback Method
hf	28.34	kJ/mol	Joback Method
hfus	16.93	kJ/mol	Joback Method
hvap	55.08	kJ/mol	Joback Method
log10ws	-1.79		Crippen Method
logp	1.280		Crippen Method
mcvol	98.860	ml/mol	McGowan Method
pc	3896.50	kPa	Joback Method
tb	570.08	K	Joback Method
tc	805.30	K	Joback Method
tf	368.95	K	Joback Method
vc	0.393	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	212.91	J/mol×K	570.08	Joback Method
cpg	221.00	J/mol×K	609.28	Joback Method
cpg	228.55	J/mol×K	648.49	Joback Method
cpg	235.58	J/mol×K	687.69	Joback Method
cpg	242.10	J/mol×K	726.90	Joback Method
cpg	248.14	J/mol×K	766.10	Joback Method
cpg	253.73	J/mol×K	805.30	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=C77326364&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