4-Amino-3-fluorobenzoic acid

Inchi: InChI=1S/C7H6FNO2/c8-5-3-4(7(10)11)1-2-6(5)9/h1-3H,9H2,(H,10,11)
InchiKey: JSKXHTHMCCDEGD-UHFFFAOYSA-N
Formula: C7H6FNO2
SMILES: Nc1ccc(C(=O)O)cc1F
Mol. weight [g/mol]: 155.13
CAS: 455-87-8

Physical Properties

Property code	Value	Unit	Source
gf	-292.89	kJ/mol	Joback Method
hf	-401.35	kJ/mol	Joback Method
hfus	21.11	kJ/mol	Joback Method
hvap	68.02	kJ/mol	Joback Method
log10ws	-1.50		Crippen Method
logp	1.106		Crippen Method
mcvol	104.920	ml/mol	McGowan Method
pc	4945.39	kPa	Joback Method
tb	614.05	K	Joback Method
tc	823.95	K	Joback Method
tf	414.71	K	Joback Method
vc	0.392	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	246.86	J/mol×K	614.05	Joback Method
cpg	254.46	J/mol×K	649.03	Joback Method
cpg	261.57	J/mol×K	684.02	Joback Method
cpg	268.22	J/mol×K	719.00	Joback Method
cpg	274.41	J/mol×K	753.98	Joback Method
cpg	280.17	J/mol×K	788.97	Joback Method
cpg	285.50	J/mol×K	823.95	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=C455878&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