2,3-Difluoroaniline

Other names: Benzenamine, 2,3-difluoro-
Inchi: InChI=1S/C6H5F2N/c7-4-2-1-3-5(9)6(4)8/h1-3H,9H2
InchiKey: YCCQGFYAVUTQFK-UHFFFAOYSA-N
Formula: C6H5F2N
SMILES: Nc1cccc(F)c1F
Mol. weight [g/mol]: 129.11
CAS: 4519-40-8

Physical Properties

Property code	Value	Unit	Source
gf	-230.38	kJ/mol	Joback Method
hf	-312.01	kJ/mol	Joback Method
hfus	15.92	kJ/mol	Joback Method
hvap	41.56	kJ/mol	Joback Method
log10ws	-1.77		Crippen Method
logp	1.547		Crippen Method
mcvol	85.160	ml/mol	McGowan Method
pc	4294.29	kPa	Joback Method
tb	444.39	K	Joback Method
tc	652.54	K	Joback Method
tf	293.28	K	Joback Method
vc	0.329	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	166.45	J/mol×K	444.39	Joback Method
cpg	174.91	J/mol×K	479.08	Joback Method
cpg	182.90	J/mol×K	513.77	Joback Method
cpg	190.45	J/mol×K	548.47	Joback Method
cpg	197.56	J/mol×K	583.16	Joback Method
cpg	204.25	J/mol×K	617.85	Joback Method
cpg	210.54	J/mol×K	652.54	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=C4519408&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