3,4-DIFLUOROANILINE

Other names: Benzenamine, 3,4-difluoro-
Inchi: InChI=1S/C6H5F2N/c7-5-2-1-4(9)3-6(5)8/h1-3H,9H2
InchiKey: AXNUZKSSQHTNPZ-UHFFFAOYSA-N
Formula: C6H5F2N
SMILES: Nc1ccc(F)c(F)c1
Mol. weight [g/mol]: 129.11

Physical Properties

Property code	Value	Unit	Source
af	0.4433		Cheméo Relay (1.0)
hf	-279.33	kJ/mol	Cheméo Relay (1.0)
hfus	15.92	kJ/mol	Joback Method
hvap	54.87	kJ/mol	Cheméo Relay (1.0)
ie	8.21	eV	Cheméo Relay (1.0)
log10ws	-1.35		Cheméo Relay (1.0)
logp	1.547		Crippen Method
mcvol	85.160	ml/mol	McGowan Method
pc	4294.29	kPa	Joback Method
tb	454.80	K	Cheméo Relay (1.0)
tc	668.61	K	Cheméo Relay (1.0)
tf	275.87	K	Cheméo Relay (1.0)

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

Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3863114&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	

Legend

af:	Acentric Factor
cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
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