Benzenamine, 2,5-difluoro-

Other names:	Aniline, 2,5-difluoro-
	2,5-Difluoroaniline
Inchi:	InChI=1S/C6H5F2N/c7-4-1-2-5(8)6(9)3-4/h1-3H,9H2
InchiKey:	YNOOQIUSYGWMSS-UHFFFAOYSA-N
Formula:	C6H5F2N
SMILES:	Nc1cc(F)ccc1F
Mol. weight [g/mol]:	129.11
CAS:	367-30-6

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	52.50 ± 0.50	kJ/mol	NIST Webbook
ie	8.41	eV	NIST Webbook
log10ws	-1.77		Crippen Method
logp	1.547		Crippen Method
mcvol	85.160	ml/mol	McGowan Method
pc	4294.29	kPa	Joback Method
tb	450.00 ± 1.00	K	NIST Webbook
tb	450.20	K	NIST Webbook
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:	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=C367306&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
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
vc:	Critical Volume