2,3,5,6-Tetrafluoroaniline

Other names: 2,3,5,6-Tetrafluoraniline
1-Amino-2,3,5,6-tetrafluorobenzene
Benzenamine, 2,3,5,6-tetrafluoro-
Aniline, 2,3,5,6-tetrafluoro-
Inchi: InChI=1S/C6H3F4N/c7-2-1-3(8)5(10)6(11)4(2)9/h1H,11H2
InchiKey: SPSWJTZNOXMMMV-UHFFFAOYSA-N
Formula: C6H3F4N
SMILES: Nc1c(F)c(F)cc(F)c1F
Mol. weight [g/mol]: 165.09
CAS: 700-17-4

Physical Properties

Property code	Value	Unit	Source
gf	-639.26	kJ/mol	Joback Method
hf	-727.17	kJ/mol	Joback Method
hfus	21.30	kJ/mol	Joback Method
hvap	41.25	kJ/mol	Joback Method
ie	8.90	eV	NIST Webbook
log10ws	-2.43		Crippen Method
logp	1.825		Crippen Method
mcvol	88.700	ml/mol	McGowan Method
pc	3690.97	kPa	Joback Method
tb	431.20	K	NIST Webbook
tb	431.00	K	NIST Webbook
tc	642.23	K	Joback Method
tf	319.50	K	Joback Method
vc	0.364	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	183.33	J/mol×K	452.89	Joback Method
cpg	190.12	J/mol×K	484.45	Joback Method
cpg	196.62	J/mol×K	516.00	Joback Method

cpg	202.83	J/mol×K	547.56	Joback Method
cpg	208.75	J/mol×K	579.12	Joback Method
cpg	214.40	J/mol×K	610.67	Joback Method
cpg	219.77	J/mol×K	642.23	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C700174&Units=SI
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

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