4-Amino-2,3,5,6-tetrafluorobenzamide

Other names:	4-Aminotetrafluorobenzamide
	Benzamide, 4-amino-2,3,5,6-tetrafluoro-
Inchi:	InChI=1S/C7H4F4N2O/c8-2-1(7(13)14)3(9)5(11)6(12)4(2)10/h12H2,(H2,13,14)
InchiKey:	CAERPAFTLPIDJT-UHFFFAOYSA-N
Formula:	C7H4F4N2O
SMILES:	NC(=O)c1c(F)c(F)c(N)c(F)c1F
Mol. weight [g/mol]:	208.11
CAS:	1548-74-9

Physical Properties

Property code	Value	Unit	Source
gf	-702.94	kJ/mol	Joback Method
hf	-838.07	kJ/mol	Joback Method
hfus	30.30	kJ/mol	Joback Method
hvap	61.52	kJ/mol	Joback Method
log10ws	-2.60		Crippen Method
logp	0.924		Crippen Method
mcvol	114.340	ml/mol	McGowan Method
pc	3731.66	kPa	Joback Method
tb	607.15	K	Joback Method
tc	813.65	K	Joback Method
tf	476.48	K	Joback Method
vc	0.456	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	276.24	J/mol×K	607.15	Joback Method
cpg	283.54	J/mol×K	641.57	Joback Method
cpg	290.44	J/mol×K	675.98	Joback Method
cpg	296.94	J/mol×K	710.40	Joback Method
cpg	303.04	J/mol×K	744.81	Joback Method
cpg	308.74	J/mol×K	779.23	Joback Method
cpg	314.04	J/mol×K	813.65	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=C1548749&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