5-Amino-2-nitrobenzotrifluoride

Other names: Benzenamine, 4-nitro-3-(trifluoromethyl)-
4-nitro-3-(trifluoromethyl)aniline
Inchi: InChI=1S/C7H5F3N2O2/c8-7(9,10)5-3-4(11)1-2-6(5)12(13)14/h1-3H,11H2
InchiKey: UTKUVRNVYFTEHF-UHFFFAOYSA-N
Formula: C7H5F3N2O2
SMILES: Nc1ccc([N+](=O)[O-])c(C(F)(F)F)c1
Mol. weight [g/mol]: 206.12
CAS: 393-11-3

Physical Properties

Property code	Value	Unit	Source
gf	-378.38	kJ/mol	Joback Method
hf	-548.27	kJ/mol	Joback Method
hfus	25.53	kJ/mol	Joback Method
hvap	58.26	kJ/mol	Joback Method
log10ws	-2.86		Crippen Method
logp	2.196		Crippen Method
mcvol	118.440	ml/mol	McGowan Method
pc	3736.23	kPa	Joback Method
tb	615.15	K	Joback Method
tc	851.35	K	Joback Method
tf	451.17	K	Joback Method
vc	0.473	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	298.10	J/mol×K	615.15	Joback Method
cpg	307.46	J/mol×K	654.52	Joback Method
cpg	315.99	J/mol×K	693.88	Joback Method
cpg	323.75	J/mol×K	733.25	Joback Method
cpg	330.80	J/mol×K	772.62	Joback Method
cpg	337.20	J/mol×K	811.98	Joback Method
cpg	343.01	J/mol×K	851.35	Joback Method

Sources

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=C393113&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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