

2-Amino-5-nitrobenzotrifluoride

Other names:	4-Nitro-a,a,a-trifluoro-o-toluidine Benzenamine, 4-nitro-2-(trifluoromethyl)- 4-nitro-«alpha», «alpha», «alpha»-trifluoro-o-toluidine
Inchi:	InChI=1S/C7H5F3N2O2/c8-7(9,10)5-3-4(12(13)14)1-2-6(5)11/h1-3H,11H2
InchiKey:	HOTZLWVITTVZGY-UHFFFAOYSA-N
Formula:	C7H5F3N2O2
SMILES:	<chem>Nc1ccc([N+](=O)[O-])cc1C(F)(F)F</chem>
Mol. weight [g/mol]:	206.12
CAS:	121-01-7

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/molxK	615.15	Joback Method
cpg	307.46	J/molxK	654.52	Joback Method
cpg	315.99	J/molxK	693.88	Joback Method
cpg	323.75	J/molxK	733.25	Joback Method
cpg	330.80	J/molxK	772.62	Joback Method
cpg	337.20	J/molxK	811.98	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C121017&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

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