

4-Fluoro-3-nitrobenzotrifluoride

Other names:	3-Nitro-4-fluoro benzotrifluoride Benzene, 1-fluoro-2-nitro-4-(trifluoromethyl)- 3-nitro-«alpha», «alpha», «alpha», 4-tetrafluorotoluene
Inchi:	InChI=1S/C7H3F4NO2/c8-5-2-1-4(7(9,10)11)3-6(5)12(13)14/h1-3H
InchiKey:	HLDFCCHSOZWKAA-UHFFFAOYSA-N
Formula:	C7H3F4NO2
SMILES:	O=[N+]([O-])c1cc(C(F)(F)F)ccc1F
Mol. weight [g/mol]:	209.10
CAS:	367-86-2

Physical Properties

Property code	Value	Unit	Source
gf	-639.64	kJ/mol	Joback Method
hf	-778.17	kJ/mol	Joback Method
hfus	23.42	kJ/mol	Joback Method
hvap	46.80	kJ/mol	Joback Method
log10ws	-3.56		Crippen Method
logp	2.753		Crippen Method
mcvol	110.230	ml/mol	McGowan Method
pc	3310.55	kPa	Joback Method
tb	541.89	K	Joback Method
tc	758.65	K	Joback Method
tf	368.50	K	Joback Method
vc	0.463	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	257.77	J/mol×K	541.89	Joback Method
cpg	267.07	J/mol×K	578.02	Joback Method
cpg	275.61	J/mol×K	614.14	Joback Method
cpg	283.45	J/mol×K	650.27	Joback Method
cpg	290.62	J/mol×K	686.40	Joback Method
cpg	297.17	J/mol×K	722.53	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	365.20	K	2.00	NIST Webbook
tbrp	365.00	K	2.00	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C367862&Units=SI
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

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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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