

4-Nitro-«alpha»,«alpha»,«alpha»-trifluorotoluene

Other names:	4-Nitrobenzotrifluoride p-Nitrobenzotrifluoride Benzene, 1-nitro-4-(trifluoromethyl)- Toluene, 4-nitro-«alpha», «alpha», «alpha»-trifluoro- p-Nitro(trifluoromethyl)benzene 4-(Trifluoromethyl)nitrobenzene 1-Nitro-4-(trifluoromethyl)benzene 4-Nitro-alpha,alpha,alpha-trifluorotoluene NSC 159121
Inchi:	InChI=1S/C7H4F3NO2/c8-7(9,10)5-1-3-6(4-2-5)11(12)13/h1-4H
InchiKey:	XKYLCLMYQDFGKO-UHFFFAOYSA-N
Formula:	C7H4F3NO2
SMILES:	O=[N+](O)c1ccc(C(F)(F)F)cc1
Mol. weight [g/mol]:	191.11
CAS:	402-54-0

Physical Properties

Property code	Value	Unit	Source
ea	1.50 ± 0.10	eV	NIST Webbook
ea	1.47 ± 0.09	eV	NIST Webbook
gf	-435.20	kJ/mol	Joback Method
hf	-570.59	kJ/mol	Joback Method
hfus	20.73	kJ/mol	Joback Method
hvap	46.96	kJ/mol	Joback Method
log10ws	-3.23		Crippen Method
logp	2.614		Crippen Method
mvol	108.460	ml/mol	McGowan Method
pc	3551.53	kPa	Joback Method
tb	537.64	K	Joback Method
tc	764.81	K	Joback Method
tf	355.39	K	Joback Method
vc	0.445	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	250.24	J/mol×K	537.64	Joback Method
cpg	260.42	J/mol×K	575.50	Joback Method
cpg	269.71	J/mol×K	613.36	Joback Method
cpg	278.17	J/mol×K	651.23	Joback Method
cpg	285.87	J/mol×K	689.09	Joback Method
cpg	292.87	J/mol×K	726.95	Joback Method
cpg	299.22	J/mol×K	764.81	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	354.50 ± 0.50	K	1.30	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C402540&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

cpg:	Ideal gas heat capacity
ea:	Electron affinity
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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