2-Nitro-«alpha»,«alpha»,«alpha»-trifluorotoluene

Other names:	o-Nitrobenzotrifluoride
	2-Nitrobenzotrifluoride
	Benzene, 1-nitro-2-(trifluoromethyl)-
	Toluene, 2-nitro-«alpha»,«alpha»,«alpha»-trifluoro-
	o-(Trifluoromethyl)nitrobenzene
	Toluene, «alpha»,«alpha»,«alpha»-trifluoro-o-nitro-
	1-Nitro-2-(trifluoromethyl)benzene
	«alpha»,«alpha»,«alpha»-Trifluoro-o-nitrotoluene
	2-(Trifluoromethyl)nitrobenzene
	o-Nitro-«alpha»,«alpha»,«alpha»-trifluorotoluene
	O-nitro-alpha,alpha,alpha-trifluorotoluene
Inchi:	InChI=1S/C7H4F3NO2/c8-7(9,10)5-3-1-2-4-6(5)11(12)13/h1-4H
InchiKey:	NDZJSUCUYPZXPR-UHFFFAOYSA-N
Formula:	C7H4F3NO2
SMILES:	O=[N+]([O-])c1ccccc1C(F)(F)F
Mol. weight [g/mol]:	191.11
CAS:	384-22-5

Physical Properties

Property code	Value	Unit	Source
ea	1.33 ± 0.10	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
mcvol	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	m3/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	377.70	K	2.70	NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C384225&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