Benzene, 1-nitro-3-(trifluoromethyl)-

Other names:	1,3-Nitrobenzotrifluoride
	1-Nitro-3-(trifluoromethyl)benzene
	3-(Trifluoromethyl)nitrobenzene
	3-Nitro-«alpha»,«alpha»,«alpha»-trifluorotoluene
	3-Nitro-Â«alphaÂ»,Â«alphaÂ»,Â«alphaÂ»-trifluorotoluene
	3-Nitrobenzotrifluoride
	NSC 10313
	Toluene, 3-nitro-«alpha»,«alpha»,«alpha»-trifluoro-
	Toluene, 3-nitro-Â«alphaÂ»,Â«alphaÂ»,Â«alphaÂ»-trifluoro-
	Toluene, «alpha»,«alpha»,«alpha»-trifluoro-m-nitro-
	Toluene, Â«alphaÂ»,Â«alphaÂ»,Â«alphaÂ»-trifluoro-m-nitro-
	USAF MA-5
	m-(Trifluoromethyl)nitrobenzene
	m-Nitro-«alpha»,«alpha»,«alpha»-trifluorotoluene
	m-Nitro-Â«alphaÂ»,Â«alphaÂ»,Â«alphaÂ»-trifluorotoluene
	m-Nitrobenzotrifluoride
	m-Nitrotrifluorotoluene
	m-Nitrotrifluortoluol
	«alpha»,«alpha»,«alpha»-Trifluoro-3-nitrotoluene
	«alpha»,«alpha»,«alpha»-Trifluoro-m-nitrotoluene
	Â«alphaÂ»,Â«alphaÂ»,Â«alphaÂ»-Trifluoro-3-nitrotoluene
	Â«alphaÂ»,Â«alphaÂ»,Â«alphaÂ»-Trifluoro-m-nitrotoluene
Inchi:	InChI=1S/C7H4F3NO2/c8-7(9,10)5-2-1-3-6(4-5)11(12)13/h1-4H
InchiKey:	WHNAMGUAXHGCHH-UHFFFAOYSA-N
Formula:	C7H4F3NO2
SMILES:	O=[N+]([O-])c1cccc(C(F)(F)F)c1
Mol. weight [g/mol]:	191.11
CAS:	98-46-4

Physical Properties

Property code	Value	Unit	Source
chl	-3228.00	kJ/mol	NIST Webbook
ea	1.41 ± 0.10	eV	NIST Webbook
ea	1.41 ± 0.05	eV	NIST Webbook
ea	1.41 ± 0.05	eV	NIST Webbook
ea	1.37 ± 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
mcvol	108.460	ml/mol	McGowan Method
pc	3551.53	kPa	Joback Method
rinpol	1032.00		NIST Webbook
tb	475.70	K	NIST Webbook
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	292.87	J/mol×K	726.95	Joback Method
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	299.22	J/mol×K	764.81	Joback Method
hvapt	53.80	kJ/mol	408.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.50327e+01
Coeff. B	-4.25388e+03
Coeff. C	-6.74670e+01
Temperature range (K), min.	355.96
Temperature range (K), max.	505.05

Sources

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=C98464&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

chl:	Standard liquid enthalpy of combustion
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
hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume