4-Nitro-3-(trifluoromethyl)phenol

Other names:	5-Hydroxy-2-nitrobenzotrifluoride Phenol, 4-nitro-3-(trifluoromethyl)- «alpha»,«alpha»,«alpha»-Trifluoro-4-nitro-m-cresol m-Cresol, «alpha»,«alpha»,«alpha»-trifluoro-4-nitro- m-Cresol, 4-nitro-«alpha»,«alpha»,«alpha»-trifluoro- Dowlap F Lamprecid Lamprecide TFM TMF USAF MA-6 3-(Trifluoromethyl)-4-nitrophenol Phenol, m-trifluoromethyl-, p-nitro- NSC 59758 1-Nitro-4-hydroxy-2-(trifluoromethyl)benzene
Inchi:	InChI=1S/C7H4F3NO3/c8-7(9,10)5-3-4(12)1-2-6(5)11(13)14/h1-3,12H
InchiKey:	ZEFMBAFMCSYJOO-UHFFFAOYSA-N
Formula:	C7H4F3NO3
SMILES:	O=[N+]([O-])c1ccc(O)cc1C(F)(F)F
Mol. weight [g/mol]:	207.11
CAS:	88-30-2

Physical Properties

Property code	Value	Unit	Source
gf	-589.82	kJ/mol	Joback Method
hf	-747.90	kJ/mol	Joback Method
hfus	26.51	kJ/mol	Joback Method
hvap	59.97	kJ/mol	Joback Method
log10ws	-2.77		Crippen Method
logp	2.319		Crippen Method
mcvol	114.330	ml/mol	McGowan Method
pc	4277.45	kPa	Joback Method
tb	618.26	K	Joback Method
tc	855.87	K	Joback Method
tf	349.00 ± 2.00	K	NIST Webbook
vc	0.410	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	290.97	J/mol×K	618.26	Joback Method
cpg	299.31	J/mol×K	657.86	Joback Method
cpg	306.84	J/mol×K	697.46	Joback Method
cpg	313.68	J/mol×K	737.07	Joback Method
cpg	319.96	J/mol×K	776.67	Joback Method
cpg	325.77	J/mol×K	816.27	Joback Method
cpg	331.26	J/mol×K	855.87	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	409.50 ± 1.50	K	0.00	NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C88302&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
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