4-Cyano-3-nitrobenzotrifluoride

Other names: Benzonitrile, 2-nitro-4-(trifluoromethyl)-
2-Nitro-4-(trifluoromethyl)benzonitrile
Inchi: InChI=1S/C8H3F3N2O2/c9-8(10,11)6-2-1-5(4-12)7(3-6)13(14)15/h1-3H
InchiKey: BQCWLXXZTCLGSZ-UHFFFAOYSA-N
Formula: C8H3F3N2O2
SMILES: N#Cc1ccc(C(F)(F)F)cc1[N+](=O)[O-]
Mol. weight [g/mol]: 216.12
CAS: 778-94-9

Physical Properties

Property code	Value	Unit	Source
gf	-303.23	kJ/mol	Joback Method
hf	-437.82	kJ/mol	Joback Method
hfus	24.43	kJ/mol	Joback Method
hvap	60.32	kJ/mol	Joback Method
log10ws	-3.58		Crippen Method
logp	2.485		Crippen Method
mcvol	123.930	ml/mol	McGowan Method
pc	3038.96	kPa	Joback Method
tb	667.58	K	Joback Method
tc	905.25	K	Joback Method
tf	444.17	K	Joback Method
vc	0.526	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	305.86	J/mol×K	667.58	Joback Method
cpg	313.69	J/mol×K	707.19	Joback Method
cpg	320.79	J/mol×K	746.80	Joback Method
cpg	327.21	J/mol×K	786.42	Joback Method
cpg	333.03	J/mol×K	826.03	Joback Method
cpg	338.29	J/mol×K	865.64	Joback Method
cpg	343.06	J/mol×K	905.25	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	430.00 ± 1.00	K	2.40	NIST Webbook

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C778949&Units=SI

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