2-Fluoro-5-nitrobenzotrifluoride

Other names: Benzene, 1-fluoro-4-nitro-2-(trifluoromethyl)-
«alpha»,«alpha»,«alpha»-2-tetrafluorotoluene
Inchi: InChI=1S/C7H3F4NO2/c8-6-2-1-4(12(13)14)3-5(6)7(9,10)11/h1-3H
InchiKey: DNTHMWUMRGOJRY-UHFFFAOYSA-N
Formula: C7H3F4NO2
SMILES: O=[N+]([O-])c1ccc(F)c(C(F)(F)F)c1
Mol. weight [g/mol]: 209.10
CAS: 400-74-8

Physical Properties

Property code	Value	Unit	Source
gf	-639.64	kJ/mol	Joback Method
hf	-778.17	kJ/mol	Joback Method
hfus	23.42	kJ/mol	Joback Method
hvap	46.80	kJ/mol	Joback Method
log10ws	-3.56		Crippen Method
logp	2.753		Crippen Method
mcvol	110.230	ml/mol	McGowan Method
pc	3310.55	kPa	Joback Method
tb	541.89	K	Joback Method
tc	758.65	K	Joback Method
tf	368.50	K	Joback Method
vc	0.463	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	257.77	J/mol×K	541.89	Joback Method
cpg	267.07	J/mol×K	578.02	Joback Method
cpg	275.61	J/mol×K	614.14	Joback Method
cpg	283.45	J/mol×K	650.27	Joback Method
cpg	290.62	J/mol×K	686.40	Joback Method
cpg	297.17	J/mol×K	722.53	Joback Method
cpg	303.15	J/mol×K	758.65	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	377.50 ± 0.50	K	2.70	NIST Webbook

Sources

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=C400748&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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