

5-Chloro-2-nitrobenzotrifluoride

Other names:	Benzene, 4-chloro-1-nitro-2-(trifluoromethyl)- 5-chloro-«alpha»,«alpha»,«alpha»-trifluoro-2-nitrotoluene
Inchi:	InChI=1S/C7H3ClF3NO2/c8-4-1-2-6(12(13)14)5(3-4)7(9,10)11/h1-3H
InchiKey:	CFPIGEXZPWTNOR-UHFFFAOYSA-N
Formula:	C7H3ClF3NO2
SMILES:	O=[N+][O-]c1ccc(Cl)cc1C(F)(F)F
Mol. weight [g/mol]:	225.55
CAS:	118-83-2

Physical Properties

Property code	Value	Unit	Source
gf	-456.76	kJ/mol	Joback Method
hf	-597.80	kJ/mol	Joback Method
hfus	24.53	kJ/mol	Joback Method
hvap	52.00	kJ/mol	Joback Method
log10ws	-3.91		Crippen Method
logp	3.267		Crippen Method
mcvol	120.700	ml/mol	McGowan Method
pc	3341.24	kPa	Joback Method
tb	496.00 ± 1.00	K	NIST Webbook
tc	812.52	K	Joback Method
tf	397.83	K	Joback Method
vc	0.493	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	270.79	J/mol×K	580.05	Joback Method
cpg	279.64	J/mol×K	618.79	Joback Method
cpg	287.69	J/mol×K	657.54	Joback Method
cpg	295.00	J/mol×K	696.28	Joback Method
cpg	301.61	J/mol×K	735.03	Joback Method
cpg	307.61	J/mol×K	773.77	Joback Method
cpg	313.02	J/mol×K	812.52	Joback Method

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=C118832&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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