2-Methoxy-5-nitrobenzotrifluoride

Other names:	5-Nitro-2-methoxybenzotrifluoride
	Benzene, 1-methoxy-4-nitro-2-(trifluoromethyl)-
	Anisole, 4-nitro-2-(trifluoromethyl)-
	4-nitro-2-(trifluoromethyl)anisole
Inchi:	InChI=1S/C8H6F3NO3/c1-15-7-3-2-5(12(13)14)4-6(7)8(9,10)11/h2-4H,1H3
InchiKey:	KGFADEJSZXEVMC-UHFFFAOYSA-N
Formula:	C8H6F3NO3
SMILES:	COc1ccc([N+](=O)[O-])cc1C(F)(F)F
Mol. weight [g/mol]:	221.13
CAS:	654-76-2

Physical Properties

Property code	Value	Unit	Source
gf	-541.41	kJ/mol	Joback Method
hf	-734.92	kJ/mol	Joback Method
hfus	24.11	kJ/mol	Joback Method
hvap	52.26	kJ/mol	Joback Method
log10ws	-3.35		Crippen Method
logp	2.622		Crippen Method
mcvol	128.420	ml/mol	McGowan Method
pc	3065.95	kPa	Joback Method
tb	587.92	K	Joback Method
tc	809.18	K	Joback Method
tf	401.41	K	Joback Method
vc	0.518	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	315.13	J/mol×K	587.92	Joback Method
cpg	325.67	J/mol×K	624.80	Joback Method
cpg	335.44	J/mol×K	661.67	Joback Method
cpg	344.46	J/mol×K	698.55	Joback Method
cpg	352.78	J/mol×K	735.42	Joback Method

cpg	360.43	J/mol×K	772.30	Joback Method
cpg	367.44	J/mol×K	809.18	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C654762&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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume