Benzene, 1,2,4-trifluoro-5-nitro-

Other names:	1,2,4-Trifluoro-5-nitrobenzene
	2,4,5-Trifluoronitrobenzene
	2,4,5-Trifluoro-1-nitrobenzene
Inchi:	InChI=1S/C6H2F3NO2/c7-3-1-5(9)6(10(11)12)2-4(3)8/h1-2H
InchiKey:	ROJNMGYMBLNTPK-UHFFFAOYSA-N
Formula:	C6H2F3NO2
SMILES:	O=[N+]([O-])c1cc(F)c(F)cc1F
Mol. weight [g/mol]:	177.08
CAS:	2105-61-5

Physical Properties

Property code	Value	Unit	Source
gf	-465.72	kJ/mol	Joback Method
hf	-564.14	kJ/mol	Joback Method
hfus	24.77	kJ/mol	Joback Method
hvap	47.35	kJ/mol	Joback Method
log10ws	-3.12		Crippen Method
logp	2.012		Crippen Method
mcvol	94.370	ml/mol	McGowan Method
pc	3759.17	kPa	Joback Method
tb	467.70	K	NIST Webbook
tc	747.12	K	Joback Method
tf	366.74	K	Joback Method
vc	0.400	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	202.84	J/mol×K	527.95	Joback Method
cpg	210.49	J/mol×K	564.48	Joback Method
cpg	217.66	J/mol×K	601.01	Joback Method
cpg	224.36	J/mol×K	637.53	Joback Method
cpg	230.62	J/mol×K	674.06	Joback Method
cpg	236.43	J/mol×K	710.59	Joback Method

cpg	241.83	J/mol×K	747.12	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2105615&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

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