3,5-Bis(trifluoromethyl)nitrobenzene

Other names:	3,5-di(Trifluoromethyl)nitrobenzene
	5-Nitro-1,3-bis(trifluoromethyl)benzene
	«alpha»,«alpha»,«alpha»,«alpha»',«alpha»',«alpha»'-Hexafluoro-5-nitro-m-xylene
	Benzene, 1-nitro-3,5-bis(trifluoromethyl)-
	«alpha»,«alpha»,«alpha»,«alpha»',«alpha»',«alpha»'-hexafluoro-5-nitroxylene
Inchi:	InChI=1S/C8H3F6NO2/c9-7(10,11)4-1-5(8(12,13)14)3-6(2-4)15(16)17/h1-3H
InchiKey:	GMUWJDVVXLBMEZ-UHFFFAOYSA-N
Formula:	C8H3F6NO2
SMILES:	O=[N+]([O-])c1cc(C(F)(F)F)cc(C(F)(F)F)c1
Mol. weight [g/mol]:	259.11
CAS:	328-75-6

Physical Properties

Property code	Value	Unit	Source
ea	1.79 ± 0.10	eV	NIST Webbook
gf	-1018.00	kJ/mol	Joback Method
hf	-1199.78	kJ/mol	Joback Method
hfus	24.75	kJ/mol	Joback Method
hvap	46.10	kJ/mol	Joback Method
log10ws	-4.33		Crippen Method
logp	3.632		Crippen Method
mcvol	127.860	ml/mol	McGowan Method
pc	2755.56	kPa	Joback Method
tb	560.08	K	Joback Method
tc	765.19	K	Joback Method
tf	383.37	K	Joback Method
vc	0.543	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	321.68	J/mol×K	560.08	Joback Method
cpg	331.51	J/mol×K	594.26	Joback Method
cpg	340.48	J/mol×K	628.45	Joback Method

cpg	348.64	J/mol×K	662.63	Joback Method
cpg	356.05	J/mol×K	696.82	Joback Method
cpg	362.79	J/mol×K	731.00	Joback Method
cpg	368.90	J/mol×K	765.19	Joback Method

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=C328756&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
ea:	Electron affinity
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