Alpha,alpha,alpha-trifluoro-4'-nitroanisole

Other names:	1-Nitro-4-(trifluoromethoxy)benzene
Inchi:	InChI=1S/C7H4F3NO3/c8-7(9,10)14-6-3-1-5(2-4-6)11(12)13/h1-4H
InchiKey:	UBEIKVUMDBCCRW-UHFFFAOYSA-N
Formula:	C7H4F3NO3
SMILES:	O=[N+]([O-])c1ccc(OC(F)(F)F)cc1
Mol. weight [g/mol]:	207.11
CAS:	713-65-5

Physical Properties

Property code	Value	Unit	Source
gf	-540.20	kJ/mol	Joback Method
hf	-702.81	kJ/mol	Joback Method
hfus	21.91	kJ/mol	Joback Method
hvap	49.37	kJ/mol	Joback Method
log10ws	-3.40		Crippen Method
logp	2.493		Crippen Method
mcvol	114.330	ml/mol	McGowan Method
pc	3480.65	kPa	Joback Method
tb	560.06	K	Joback Method
tc	784.37	K	Joback Method
tf	377.62	K	Joback Method
vc	0.463	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	271.67	J/mol×K	560.06	Joback Method
cpg	281.58	J/mol×K	597.45	Joback Method
cpg	290.70	J/mol×K	634.83	Joback Method
cpg	299.06	J/mol×K	672.22	Joback Method
cpg	306.71	J/mol×K	709.60	Joback Method
cpg	313.69	J/mol×K	746.99	Joback Method
cpg	320.04	J/mol×K	784.37	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C713655&Units=SI

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