2,3,6-Trifluorobenzonitrile

Inchi: InChI=1S/C7H2F3N/c8-5-1-2-6(9)7(10)4(5)3-11/h1-2H
InchiKey: YWTXHALVWAISPR-UHFFFAOYSA-N
Formula: C7H2F3N
SMILES: N#Cc1c(F)ccc(F)c1F
Mol. weight [g/mol]: 157.09
CAS: 136514-17-5

Physical Properties

Property code	Value	Unit	Source
gf	-359.67	kJ/mol	Joback Method
hf	-409.14	kJ/mol	Joback Method
hfus	17.51	kJ/mol	Joback Method
hvap	43.47	kJ/mol	Joback Method
log10ws	-2.82		Crippen Method
logp	1.976		Crippen Method
mcvol	92.420	ml/mol	McGowan Method
pc	3213.68	kPa	Joback Method
tb	501.07	K	Joback Method
tc	705.21	K	Joback Method
tf	299.39	K	Joback Method
vc	0.400	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	184.66	J/mol×K	501.07	Joback Method
cpg	191.32	J/mol×K	535.09	Joback Method
cpg	197.63	J/mol×K	569.12	Joback Method
cpg	203.60	J/mol×K	603.14	Joback Method
cpg	209.23	J/mol×K	637.16	Joback Method
cpg	214.54	J/mol×K	671.18	Joback Method
cpg	219.52	J/mol×K	705.21	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=C136514175&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