2,3,4-Trifluoroaniline

Inchi: InChI=1S/C6H4F3N/c7-3-1-2-4(10)6(9)5(3)8/h1-2H,10H2
InchiKey: WRDGNXCXTDDYBZ-UHFFFAOYSA-N
Formula: C6H4F3N
SMILES: Nc1ccc(F)c(F)c1F
Mol. weight [g/mol]: 147.10
CAS: 3862-73-5

Physical Properties

Property code	Value	Unit	Source
gf	-434.82	kJ/mol	Joback Method
hf	-519.59	kJ/mol	Joback Method
hfus	18.61	kJ/mol	Joback Method
hvap	53.70 ± 0.50	kJ/mol	NIST Webbook
log10ws	-2.10		Crippen Method
logp	1.686		Crippen Method
mcvol	86.930	ml/mol	McGowan Method
pc	3975.52	kPa	Joback Method
tb	448.64	K	Joback Method
tc	647.02	K	Joback Method
tf	306.39	K	Joback Method
vc	0.346	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	174.95	J/mol×K	448.64	Joback Method
cpg	182.53	J/mol×K	481.70	Joback Method
cpg	189.75	J/mol×K	514.77	Joback Method
cpg	196.60	J/mol×K	547.83	Joback Method
cpg	203.09	J/mol×K	580.89	Joback Method
cpg	209.25	J/mol×K	613.96	Joback Method
cpg	215.06	J/mol×K	647.02	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	365.00	K	6.40	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3862735&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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume