2,3,6-Trifluorophenol

Inchi: InChI=1S/C6H3F3O/c7-3-1-2-4(8)6(10)5(3)9/h1-2,10H
InchiKey: QSFGUSFDWCVXNR-UHFFFAOYSA-N
Formula: C6H3F3O
SMILES: Oc1c(F)ccc(F)c1F
Mol. weight [g/mol]: 148.08
CAS: 113798-74-6

Physical Properties

Property code	Value	Unit	Source
gf	-646.26	kJ/mol	Joback Method
hf	-719.22	kJ/mol	Joback Method
hfus	19.58	kJ/mol	Joback Method
hvap	43.11	kJ/mol	Joback Method
log10ws	-2.01		Crippen Method
logp	1.810		Crippen Method
mcvol	82.820	ml/mol	McGowan Method
pc	4571.55	kPa	Joback Method
tb	451.75	K	Joback Method
tc	651.70	K	Joback Method
tf	322.33	K	Joback Method
vc	0.283	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	171.14	J/mol×K	451.75	Joback Method
cpg	178.30	J/mol×K	485.08	Joback Method
cpg	184.94	J/mol×K	518.40	Joback Method
cpg	191.10	J/mol×K	551.73	Joback Method
cpg	196.82	J/mol×K	585.05	Joback Method
cpg	202.14	J/mol×K	618.38	Joback Method
cpg	207.11	J/mol×K	651.70	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=C113798746&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