2,4,6-Trifluorobenzoic acid

Inchi: InChI=1S/C7H3F3O2/c8-3-1-4(9)6(7(11)12)5(10)2-3/h1-2H,(H,11,12)
InchiKey: SJZATRRXUILGHH-UHFFFAOYSA-N
Formula: C7H3F3O2
SMILES: O=C(O)c1c(F)cc(F)cc1F
Mol. weight [g/mol]: 176.09
CAS: 28314-80-9

Physical Properties

Property code	Value	Unit	Source
gf	-758.59	kJ/mol	Joback Method
hf	-838.83	kJ/mol	Joback Method
hfus	21.69	kJ/mol	Joback Method
hvap	56.41	kJ/mol	Joback Method
log10ws	-2.53		Crippen Method
logp	1.802		Crippen Method
mcvol	98.480	ml/mol	McGowan Method
pc	3985.56	kPa	Joback Method
tb	545.04	K	Joback Method
tc	729.27	K	Joback Method
tf	345.15	K	Joback Method
vc	0.399	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	216.12	J/mol×K	545.04	Joback Method
cpg	222.66	J/mol×K	575.75	Joback Method
cpg	228.86	J/mol×K	606.45	Joback Method
cpg	234.74	J/mol×K	637.16	Joback Method
cpg	240.29	J/mol×K	667.86	Joback Method
cpg	245.53	J/mol×K	698.57	Joback Method
cpg	250.46	J/mol×K	729.27	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=C28314809&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