Tetronic acid, trifluoroacetate

Inchi: InChI=1S/C6H3F3O4/c7-6(8,9)5(11)13-3-1-4(10)12-2-3/h1H,2H2
InchiKey: GWLYACFXDZCQTH-UHFFFAOYSA-N
Formula: C6H3F3O4
SMILES: O=C1C=C(OC(=O)C(F)(F)F)CO1
Mol. weight [g/mol]: 196.08

Physical Properties

Property code	Value	Unit	Source
gf	-959.99	kJ/mol	Joback Method
hf	-1151.62	kJ/mol	Joback Method
hfus	17.10	kJ/mol	Joback Method
hvap	44.64	kJ/mol	Joback Method
log10ws	-0.97		Crippen Method
logp	0.533		Crippen Method
mcvol	100.430	ml/mol	McGowan Method
pc	3886.79	kPa	Joback Method
rinpol	996.00		NIST Webbook
rinpol	996.00		NIST Webbook
tb	526.41	K	Joback Method
tc	734.88	K	Joback Method
tf	356.94	K	Joback Method
vc	0.395	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	239.98	J/mol×K	526.41	Joback Method
cpg	249.17	J/mol×K	561.16	Joback Method
cpg	257.82	J/mol×K	595.90	Joback Method
cpg	265.94	J/mol×K	630.65	Joback Method
cpg	273.53	J/mol×K	665.39	Joback Method
cpg	280.59	J/mol×K	700.14	Joback Method
cpg	287.13	J/mol×K	734.88	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=U376222&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume