Tetronic acid, heptafluorobutyrate

Inchi: InChI=1S/C8H3F7O4/c9-6(10,7(11,12)8(13,14)15)5(17)19-3-1-4(16)18-2-3/h1H,2H2
InchiKey: SBEGGRFGQKHHNJ-UHFFFAOYSA-N
Formula: C8H3F7O4
SMILES: O=C1C=C(OC(=O)C(F)(F)C(F)(F)C(F)(F)F)CO1
Mol. weight [g/mol]: 296.10

Physical Properties

Property code	Value	Unit	Source
gf	-1716.71	kJ/mol	Joback Method
hf	-1994.84	kJ/mol	Joback Method
hfus	19.77	kJ/mol	Joback Method
hvap	43.23	kJ/mol	Joback Method
log10ws	-2.43		Crippen Method
logp	1.803		Crippen Method
mcvol	135.690	ml/mol	McGowan Method
pc	2662.52	kPa	Joback Method
rinpol	1048.00		NIST Webbook
rinpol	1048.00		NIST Webbook
tb	562.79	K	Joback Method
tc	750.77	K	Joback Method
tf	386.68	K	Joback Method
vc	0.556	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	368.08	J/mol×K	562.79	Joback Method
cpg	378.40	J/mol×K	594.12	Joback Method
cpg	387.93	J/mol×K	625.45	Joback Method
cpg	396.71	J/mol×K	656.78	Joback Method
cpg	404.79	J/mol×K	688.11	Joback Method
cpg	412.19	J/mol×K	719.44	Joback Method
cpg	418.95	J/mol×K	750.77	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U376223&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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