Tetrafluorophthalic acid

Other names: 1,2-Benzenedicarboxylic acid, 3,4,5,6-tetrafluoro-
3,4,5,6-tetrafluorophthalic acid
Inchi: InChI=1S/C8H2F4O4/c9-3-1(7(13)14)2(8(15)16)4(10)6(12)5(3)11/h(H,13,14)(H,15,16)
InchiKey: YJLVXRPNNDKMMO-UHFFFAOYSA-N
Formula: C8H2F4O4
SMILES: O=C(O)c1c(F)c(F)c(F)c(F)c1C(=O)O
Mol. weight [g/mol]: 238.09
CAS: 652-03-9

Physical Properties

Property code	Value	Unit	Source
gf	-1229.98	kJ/mol	Joback Method
hf	-1343.33	kJ/mol	Joback Method
hfus	32.27	kJ/mol	Joback Method
hvap	82.57	kJ/mol	Joback Method
log10ws	-2.92		Crippen Method
logp	1.639		Crippen Method
mcvol	121.780	ml/mol	McGowan Method
pc	3906.25	kPa	Joback Method
tb	723.20	K	Joback Method
tc	903.55	K	Joback Method
tf	492.80	K	Joback Method
vc	0.497	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	306.50	J/mol×K	723.20	Joback Method
cpg	311.65	J/mol×K	753.26	Joback Method
cpg	316.48	J/mol×K	783.32	Joback Method
cpg	320.99	J/mol×K	813.38	Joback Method
cpg	325.18	J/mol×K	843.43	Joback Method
cpg	329.07	J/mol×K	873.49	Joback Method
cpg	332.63	J/mol×K	903.55	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=C652039&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