2,3,5,6-Tetrafluoroanisole

Other names:	2,3,5,6-Tetrafluoromethoxybenzene
	Benzene, 1,2,4,5-tetrafluoro-3-methoxy-
	Anisole, 2,3,5,6-tetrafluoro-
	1,2,4,5-Tetrafluoro-3-methoxybenzene
Inchi:	InChI=1S/C7H4F4O/c1-12-7-5(10)3(8)2-4(9)6(7)11/h2H,1H3
InchiKey:	AXCOCGJDERQVDK-UHFFFAOYSA-N
Formula:	C7H4F4O
SMILES:	COc1c(F)c(F)cc(F)c1F
Mol. weight [g/mol]:	180.10
CAS:	2324-98-3

Physical Properties

Property code	Value	Unit	Source
ea	0.22 ± 0.09	eV	NIST Webbook
gf	-802.29	kJ/mol	Joback Method
hf	-913.82	kJ/mol	Joback Method
hfus	19.88	kJ/mol	Joback Method
hvap	35.24	kJ/mol	Joback Method
log10ws	-2.92		Crippen Method
logp	2.252		Crippen Method
mcvol	98.680	ml/mol	McGowan Method
pc	3032.27	kPa	Joback Method
tb	411.20	K	NIST Webbook
tc	599.90	K	Joback Method
tf	269.74	K	Joback Method
vc	0.409	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	196.49	J/mol×K	425.66	Joback Method
cpg	203.76	J/mol×K	454.70	Joback Method
cpg	210.82	J/mol×K	483.74	Joback Method
cpg	217.67	J/mol×K	512.78	Joback Method

cpg	224.30	J/mol×K	541.82	Joback Method
cpg	230.72	J/mol×K	570.86	Joback Method
cpg	236.91	J/mol×K	599.90	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2324983&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
ea:	Electron affinity
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