Pentafluoroanisole

Other names:	Pentafluoroanisole
	2,3,4,5,6-Pentafluoroanisole
	Anisole, 2,3,4,5,6-pentafluoro-
	Methyl pentafluorophenyl ether
	Pentafluorophenyl methyl ether
Inchi:	InChI=1S/C7H3F5O/c1-13-7-5(11)3(9)2(8)4(10)6(7)12/h1H3
InchiKey:	ZRQUIRABLIQJRI-UHFFFAOYSA-N
Formula:	C7H3F5O
SMILES:	COc1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]:	198.09

Physical Properties

Property code	Value	Unit	Source
ea	0.54 ± 0.09	eV	NIST Webbook
hfus	22.57	kJ/mol	Joback Method
ie	9.10 ± 0.02	eV	NIST Webbook
logp	2.391		Crippen Method
mcvol	100.450	ml/mol	McGowan Method
tb	411.00	K	NIST Webbook
tb	411.70	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	205.28	J/mol×K	429.91	Joback Method
cpg	211.81	J/mol×K	457.70	Joback Method
cpg	218.20	J/mol×K	485.50	Joback Method
cpg	224.42	J/mol×K	513.29	Joback Method
cpg	230.49	J/mol×K	541.08	Joback Method
cpg	236.38	J/mol×K	568.87	Joback Method
cpg	242.09	J/mol×K	596.67	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C389402&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
ea:	Electron affinity
hfus:	Enthalpy of fusion at standard conditions
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature

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