Pentafluoropropanoic acid methyl ester

Other names:	Methyl pentafluoropropionate
	Methyl pentafluoropropanoate
	Propanoic acid, pentafluoro-, methyl ester
	Propionic acid, pentafluoro-, methyl ester
	Methylester kyseliny pentafluorpropionove
	Pentafluoropropionic acid methyl ester
	Perfluoropropionic acid, methyl ester
	2,2,3,3,3-Pentafluoro-propionic acid methyl ester
Inchi:	InChI=1S/C4H3F5O2/c1-11-2(10)3(5,6)4(7,8)9/h1H3
InchiKey:	JMKJCPUVEMZGEC-UHFFFAOYSA-N
Formula:	C4H3F5O2
SMILES:	COC(=O)C(F)(F)C(F)(F)F
Mol. weight [g/mol]:	178.06
CAS:	378-75-6

Physical Properties

Property code	Value	Unit	Source
chl	-1434.60 ± 1.70	kJ/mol	NIST Webbook
gf	-1219.49	kJ/mol	Joback Method
hf	-1428.30 ± 2.80	kJ/mol	NIST Webbook
hfl	-1463.00 ± 1.80	kJ/mol	NIST Webbook
hfus	9.47	kJ/mol	Joback Method
hvap	35.00	kJ/mol	NIST Webbook
log10ws	-1.34		Crippen Method
logp	1.357		Crippen Method
mcvol	83.510	ml/mol	McGowan Method
pc	3291.59	kPa	Joback Method
rinpol	437.00		NIST Webbook
rinpol	437.20		NIST Webbook
tb	332.50 ± 0.50	K	NIST Webbook
tc	511.61	K	Joback Method
tf	214.79	K	Joback Method
vc	0.351	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	173.16	J/mol×K	357.10	Joback Method
cpg	180.89	J/mol×K	382.85	Joback Method
cpg	188.19	J/mol×K	408.60	Joback Method
cpg	195.07	J/mol×K	434.36	Joback Method
cpg	201.56	J/mol×K	460.11	Joback Method
cpg	207.66	J/mol×K	485.86	Joback Method
cpg	213.39	J/mol×K	511.61	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	334.20	K	98.50	NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C378756&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

Legend

chl: Standard liquid enthalpy of combustion
cpg: Ideal gas heat capacity
gf: Standard Gibbs free energy of formation
hf: Enthalpy of formation at standard conditions
hfl: Liquid phase 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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume