Methyl pentafluorobenzoate

Other names: Pentafluorobenzoic acid, methyl ester
Inchi: InChI=1S/C8H3F5O2/c1-15-8(14)2-3(9)5(11)7(13)6(12)4(2)10/h1H3
InchiKey: UXJRQNXHCZKHRJ-UHFFFAOYSA-N
Formula: C8H3F5O2
SMILES: COC(=O)c1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]: 226.10
CAS: 36629-42-2

Physical Properties

Property code	Value	Unit	Source
gf	-1127.23	kJ/mol	Joback Method
hf	-1254.62	kJ/mol	Joback Method
hfus	26.76	kJ/mol	Joback Method
hvap	44.06	kJ/mol	Joback Method
log10ws	-3.37		Crippen Method
logp	2.169		Crippen Method
mcvol	116.110	ml/mol	McGowan Method
pc	2744.03	kPa	Joback Method
rinpol	946.00		NIST Webbook
rinpol	956.00		NIST Webbook
rinpol	943.00		NIST Webbook
rinpol	949.00		NIST Webbook
rinpol	992.00		NIST Webbook
rinpol	946.00		NIST Webbook
rinpol	982.00		NIST Webbook
rinpol	957.00		NIST Webbook
ripol	1299.00		NIST Webbook
ripol	1305.00		NIST Webbook
ripol	1308.00		NIST Webbook
ripol	1353.00		NIST Webbook
ripol	1325.00		NIST Webbook
ripol	1352.00		NIST Webbook
ripol	1260.00		NIST Webbook
tb	506.66	K	Joback Method
tc	682.22	K	Joback Method
tf	344.05	K	Joback Method
vc	0.489	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	254.56	J/mol×K	506.66	Joback Method
cpg	261.92	J/mol×K	535.92	Joback Method
cpg	269.04	J/mol×K	565.18	Joback Method
cpg	275.90	J/mol×K	594.44	Joback Method
cpg	282.51	J/mol×K	623.70	Joback Method
cpg	288.86	J/mol×K	652.96	Joback Method
cpg	294.93	J/mol×K	682.22	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C36629422&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
ripol: Polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature

tf: Normal melting (fusion) point

vc: Critical Volume

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