Pentafluorobenzoic acid, ethyl ester

Other names:	Benzoic acid, pentafluoro-, ethyl ester
	Pentafluorobenzoic acid, ethyl ester
	Benzoic acid, 2,3,4,5,6-pentafluoro-, ethyl ester
	ethyl perfluorobenzoate
Inchi:	InChI=1S/C9H5F5O2/c1-2-16-9(15)3-4(10)6(12)8(14)7(13)5(3)11/h2H2,1H3
InchiKey:	DFUDMSIRGGTHGI-UHFFFAOYSA-N
Formula:	C9H5F5O2
SMILES:	CCOC(=O)c1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]:	240.13

Physical Properties

Property code	Value	Unit	Source
af	0.5704		Cheméo Relay (1.0)
gf	-1118.81	kJ/mol	Joback Method
hf	-1115.38	kJ/mol	Cheméo Relay (1.0)
hfus	29.35	kJ/mol	Joback Method
hvap	61.57	kJ/mol	Cheméo Relay (1.0)
ie	10.05	eV	NIST Webbook
log10ws	-4.85		Cheméo Relay (1.0)
logp	2.559		Crippen Method
mcvol	130.200	ml/mol	McGowan Method
pc	2487.55	kPa	Joback Method
rinpol	1071.00		NIST Webbook
rinpol	1025.00		NIST Webbook
rinpol	1032.00		NIST Webbook
rinpol	1055.00		NIST Webbook
rinpol	1025.00		NIST Webbook
rinpol	1024.00		NIST Webbook
rinpol	1017.00		NIST Webbook
rinpol	1033.00		NIST Webbook
rinpol	1024.00		NIST Webbook
ripol	1381.00		NIST Webbook
ripol	1383.00		NIST Webbook
ripol	1351.00		NIST Webbook
ripol	1381.00		NIST Webbook
ripol	1328.00		NIST Webbook
ripol	1347.00		NIST Webbook

ripol	1343.00		NIST Webbook
tb	463.59	K	Cheméo Relay (1.0)
tc	645.74	K	Cheméo Relay (1.0)
tf	264.94	K	Cheméo Relay (1.0)
vc	0.498	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	296.24	J/mol×K	529.54	Joback Method
cpg	304.70	J/mol×K	558.55	Joback Method
cpg	312.86	J/mol×K	587.57	Joback Method
cpg	320.70	J/mol×K	616.58	Joback Method
cpg	328.24	J/mol×K	645.59	Joback Method
cpg	335.45	J/mol×K	674.61	Joback Method
cpg	342.34	J/mol×K	703.62	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=C4522934&Units=SI
Joback Method: https://en.wikipedia.org/wiki/Joback_method

Legend

af: Acentric Factor
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

ie:	Ionization energy
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