Propanoic acid, pentafluoro-, ethyl ester

Other names:	Ethyl perfluoropropionate
	Ethyl pentafluoropropionate
	2,2,3,3,3-Pentafluoro-propionic acid ethyl ester
	Ethyl pentafluoropentanoate
	Pentafluoropropionic acid, ethyl ester
Inchi:	InChI=1S/C5H5F5O2/c1-2-12-3(11)4(6,7)5(8,9)10/h2H2,1H3
InchiKey:	DBOFMRQAMAZKQY-UHFFFAOYSA-N
Formula:	C5H5F5O2
SMILES:	CCOC(=O)C(F)(F)C(F)(F)F
Mol. weight [g/mol]:	192.08
CAS:	426-65-3

Physical Properties

Property code	Value	Unit	Source
gf	-1211.07	kJ/mol	Joback Method
hf	-1389.38	kJ/mol	Joback Method
hfus	12.06	kJ/mol	Joback Method
hvap	29.20	kJ/mol	Joback Method
log10ws	-1.75		Crippen Method
logp	1.747		Crippen Method
mcvol	97.600	ml/mol	McGowan Method
pc	2956.90	kPa	Joback Method
rinpol	510.00		NIST Webbook
rinpol	510.40		NIST Webbook
rinpol	510.00		NIST Webbook
tb	348.50 ± 0.50	K	NIST Webbook
tb	348.70	K	NIST Webbook
tc	534.69	K	Joback Method
tf	226.06	K	Joback Method
vc	0.407	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	208.03	J/mol×K	379.98	Joback Method
cpg	216.88	J/mol×K	405.76	Joback Method
cpg	225.26	J/mol×K	431.55	Joback Method
cpg	233.18	J/mol×K	457.33	Joback Method
cpg	240.66	J/mol×K	483.12	Joback Method
cpg	247.72	J/mol×K	508.90	Joback Method
cpg	254.37	J/mol×K	534.69	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C426653&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume