Ethyl perfluoropentanoate

Other names: 2,2,3,3,4,4,5,5,5-Nonafluoro-pentanoic acid ethyl ester
Inchi: InChI=1S/C7H5F9O2/c1-2-18-3(17)4(8,9)5(10,11)6(12,13)7(14,15)16/h2H2,1H3
InchiKey: JBEYNXOZKKQLOH-UHFFFAOYSA-N
Formula: C7H5F9O2
SMILES: CCOC(=O)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 292.10

Physical Properties

Property code	Value	Unit	Source
gf	-1967.79	kJ/mol	Joback Method
hf	-2232.60	kJ/mol	Joback Method
hfus	14.74	kJ/mol	Joback Method
hvap	27.79	kJ/mol	Joback Method
log10ws	-3.22		Crippen Method
logp	3.018		Crippen Method
mcvol	132.860	ml/mol	McGowan Method
pc	2117.78	kPa	Joback Method
rinpol	612.00		NIST Webbook
rinpol	611.50		NIST Webbook
rinpol	612.00		NIST Webbook
tb	416.36	K	Joback Method
tc	558.89	K	Joback Method
tf	255.80	K	Joback Method
vc	0.570	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	321.41	J/mol×K	416.36	Joback Method
cpg	332.52	J/mol×K	440.11	Joback Method
cpg	342.96	J/mol×K	463.87	Joback Method
cpg	352.73	J/mol×K	487.62	Joback Method
cpg	361.88	J/mol×K	511.38	Joback Method
cpg	370.44	J/mol×K	535.13	Joback Method

cpg	378.42	J/mol×K	558.89	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R70101&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

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