2,2,3,3,4,4,5,5,5-Nonafluoro-pentanoic acid methyl ester

Other names: Methyl perfluoropentanoate
Inchi: InChI=1S/C6H3F9O2/c1-17-2(16)3(7,8)4(9,10)5(11,12)6(13,14)15/h1H3
InchiKey: OSDPSOBLGQUCQX-UHFFFAOYSA-N
Formula: C6H3F9O2
SMILES: COC(=O)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 278.07

Physical Properties

Property code	Value	Unit	Source
gf	-1976.21	kJ/mol	Joback Method
hf	-2211.96	kJ/mol	Joback Method
hfus	12.15	kJ/mol	Joback Method
hvap	25.57	kJ/mol	Joback Method
log10ws	-2.80		Crippen Method
logp	2.628		Crippen Method
mcvol	118.770	ml/mol	McGowan Method
pc	2318.07	kPa	Joback Method
rinpol	538.60		NIST Webbook
rinpol	539.00		NIST Webbook
rinpol	539.00		NIST Webbook
tb	393.48	K	Joback Method
tc	535.72	K	Joback Method
tf	244.53	K	Joback Method
vc	0.513	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	281.26	J/mol×K	393.48	Joback Method
cpg	291.69	J/mol×K	417.19	Joback Method
cpg	301.46	J/mol×K	440.89	Joback Method
cpg	310.59	J/mol×K	464.60	Joback Method
cpg	319.11	J/mol×K	488.30	Joback Method
cpg	327.05	J/mol×K	512.01	Joback Method

cpg	334.44	J/mol×K	535.72	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R70183&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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