Methyl perfluorohexanoate

Other names: 2,2,3,3,4,4,5,5,6,6,6-Undecafluoro- hexanoic acid methyl ester
Inchi: InChI=1S/C7H3F11O2/c1-20-2(19)3(8,9)4(10,11)5(12,13)6(14,15)7(16,17)18/h1H3
InchiKey: NJXMLQHJFDKLKL-UHFFFAOYSA-N
Formula: C7H3F11O2
SMILES: COC(=O)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 328.08

Physical Properties

Property code	Value	Unit	Source
gf	-2354.57	kJ/mol	Joback Method
hf	-2633.57	kJ/mol	Joback Method
hfus	13.48	kJ/mol	Joback Method
hvap	24.87	kJ/mol	Joback Method
log10ws	-3.53		Crippen Method
logp	3.263		Crippen Method
mcvol	136.400	ml/mol	McGowan Method
pc	1985.89	kPa	Joback Method
rinpol	596.00		NIST Webbook
rinpol	595.70		NIST Webbook
rinpol	596.00		NIST Webbook
tb	411.67	K	Joback Method
tc	548.72	K	Joback Method
tf	259.40	K	Joback Method
vc	0.595	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	339.47	J/mol×K	411.67	Joback Method
cpg	350.78	J/mol×K	434.51	Joback Method
cpg	361.35	J/mol×K	457.35	Joback Method
cpg	371.22	J/mol×K	480.19	Joback Method
cpg	380.41	J/mol×K	503.03	Joback Method
cpg	388.95	J/mol×K	525.88	Joback Method

cpg	396.88	J/mol×K	548.72	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R70179&Units=SI

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