2,2,3,3,4,4,5,5,6,6,6-Undecafluoro- hexanoic acid propyl ester

Other names: Propyl perfluorohexanoate
Inchi: InChI=1S/C9H7F11O2/c1-2-3-22-4(21)5(10,11)6(12,13)7(14,15)8(16,17)9(18,19)20/h2-3
InchiKey: UFTXWKSBYSWRLM-UHFFFAOYSA-N
Formula: C9H7F11O2
SMILES: CCCOC(=O)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 356.13

Physical Properties

Property code	Value	Unit	Source
gf	-2337.73	kJ/mol	Joback Method
hf	-2674.85	kJ/mol	Joback Method
hfus	18.66	kJ/mol	Joback Method
hvap	29.32	kJ/mol	Joback Method
log10ws	-4.37		Crippen Method
logp	4.043		Crippen Method
mcvol	164.580	ml/mol	McGowan Method
pc	1685.18	kPa	Joback Method
rinpol	750.00		NIST Webbook
rinpol	750.50		NIST Webbook
rinpol	750.00		NIST Webbook
tb	457.43	K	Joback Method
tc	595.37	K	Joback Method
tf	281.94	K	Joback Method
vc	0.707	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	425.99	J/mol×K	457.43	Joback Method
cpg	438.30	J/mol×K	480.42	Joback Method
cpg	449.85	J/mol×K	503.41	Joback Method
cpg	460.66	J/mol×K	526.40	Joback Method
cpg	470.78	J/mol×K	549.39	Joback Method
cpg	480.23	J/mol×K	572.38	Joback Method

cpg	489.05	J/mol×K	595.37	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R70268&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