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

Other names: Propyl perfluoropentanoate
Inchi: InChI=1S/C8H7F9O2/c1-2-3-19-4(18)5(9,10)6(11,12)7(13,14)8(15,16)17/h2-3H2,1H3
InchiKey: CQTLZOHQVZFPOE-UHFFFAOYSA-N
Formula: C8H7F9O2
SMILES: CCCOC(=O)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 306.13

Physical Properties

Property code	Value	Unit	Source
gf	-1959.37	kJ/mol	Joback Method
hf	-2253.24	kJ/mol	Joback Method
hfus	17.33	kJ/mol	Joback Method
hvap	30.02	kJ/mol	Joback Method
log10ws	-3.64		Crippen Method
logp	3.408		Crippen Method
mcvol	146.950	ml/mol	McGowan Method
pc	1942.37	kPa	Joback Method
rinpol	696.00		NIST Webbook
rinpol	695.60		NIST Webbook
rinpol	696.00		NIST Webbook
tb	439.24	K	Joback Method
tc	581.96	K	Joback Method
tf	267.07	K	Joback Method
vc	0.625	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	363.46	J/mol×K	439.24	Joback Method
cpg	375.20	J/mol×K	463.03	Joback Method
cpg	386.23	J/mol×K	486.81	Joback Method
cpg	396.59	J/mol×K	510.60	Joback Method
cpg	406.32	J/mol×K	534.39	Joback Method
cpg	415.42	J/mol×K	558.18	Joback Method

cpg	423.95	J/mol×K	581.96	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=R70272&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

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