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

Other names: Butyl perfluoropentanoate
Inchi: InChI=1S/C9H9F9O2/c1-2-3-4-20-5(19)6(10,11)7(12,13)8(14,15)9(16,17)18/h2-4H2,1H3
InchiKey: MPAULUFXCUVYQJ-UHFFFAOYSA-N
Formula: C9H9F9O2
SMILES: CCCCOC(=O)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 320.15

Physical Properties

Property code	Value	Unit	Source
gf	-1950.95	kJ/mol	Joback Method
hf	-2273.88	kJ/mol	Joback Method
hfus	19.92	kJ/mol	Joback Method
hvap	32.25	kJ/mol	Joback Method
log10ws	-4.06		Crippen Method
logp	3.798		Crippen Method
mcvol	161.040	ml/mol	McGowan Method
pc	1787.88	kPa	Joback Method
rinpol	787.00		NIST Webbook
rinpol	787.30		NIST Webbook
tb	462.12	K	Joback Method
tc	605.02	K	Joback Method
tf	278.34	K	Joback Method
vc	0.681	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	407.31	J/mol×K	462.12	Joback Method
cpg	419.61	J/mol×K	485.94	Joback Method
cpg	431.19	J/mol×K	509.75	Joback Method
cpg	442.09	J/mol×K	533.57	Joback Method
cpg	452.33	J/mol×K	557.38	Joback Method
cpg	461.95	J/mol×K	581.20	Joback Method
cpg	470.97	J/mol×K	605.02	Joback Method

Sources

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=R70062&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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