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

Other names: Pentyl perfluoropentanoate
Inchi: InChI=1S/C10H11F9O2/c1-2-3-4-5-21-6(20)7(11,12)8(13,14)9(15,16)10(17,18)19/h2-5H
InchiKey: CONLYJQXVPYISQ-UHFFFAOYSA-N
Formula: C10H11F9O2
SMILES: CCCCCOC(=O)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 334.18

Physical Properties

Property code	Value	Unit	Source
gf	-1942.53	kJ/mol	Joback Method
hf	-2294.52	kJ/mol	Joback Method
hfus	22.51	kJ/mol	Joback Method
hvap	34.47	kJ/mol	Joback Method
log10ws	-4.48		Crippen Method
logp	4.188		Crippen Method
mcvol	175.130	ml/mol	McGowan Method
pc	1651.11	kPa	Joback Method
rinpol	882.00		NIST Webbook
rinpol	881.60		NIST Webbook
rinpol	882.00		NIST Webbook
tb	485.00	K	Joback Method
tc	628.11	K	Joback Method
tf	289.61	K	Joback Method
vc	0.738	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	452.87	J/mol×K	485.00	Joback Method
cpg	465.68	J/mol×K	508.85	Joback Method
cpg	477.77	J/mol×K	532.70	Joback Method
cpg	489.15	J/mol×K	556.55	Joback Method
cpg	499.87	J/mol×K	580.41	Joback Method
cpg	509.95	J/mol×K	604.26	Joback Method

cpg	519.42	J/mol×K	628.11	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R70222&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