Hexyl perfluoropentanoate

Other names: 2,2,3,3,4,4,5,5,5-Nonafluoro-pentanoic acid hexyl ester
Inchi: InChI=1S/C11H13F9O2/c1-2-3-4-5-6-22-7(21)8(12,13)9(14,15)10(16,17)11(18,19)20/h2-
InchiKey: FALKAIRAHKEYPI-UHFFFAOYSA-N
Formula: C11H13F9O2
SMILES: CCCCCCOC(=O)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 348.21

Physical Properties

Property code	Value	Unit	Source
gf	-1934.11	kJ/mol	Joback Method
hf	-2315.16	kJ/mol	Joback Method
hfus	25.10	kJ/mol	Joback Method
hvap	36.70	kJ/mol	Joback Method
log10ws	-4.89		Crippen Method
logp	4.578		Crippen Method
mcvol	189.220	ml/mol	McGowan Method
pc	1529.46	kPa	Joback Method
rinpol	976.90		NIST Webbook
rinpol	977.00		NIST Webbook
tb	507.88	K	Joback Method
tc	651.30	K	Joback Method
tf	300.88	K	Joback Method
vc	0.793	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	500.04	J/mol×K	507.88	Joback Method
cpg	513.33	J/mol×K	531.78	Joback Method
cpg	525.87	J/mol×K	555.69	Joback Method
cpg	537.71	J/mol×K	579.59	Joback Method
cpg	548.86	J/mol×K	603.50	Joback Method
cpg	559.36	J/mol×K	627.40	Joback Method
cpg	569.25	J/mol×K	651.30	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R70151&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

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