Heptadecafluorononanoic acid, pentyl ester

Inchi: InChI=1S/C14H11F17O2/c1-2-3-4-5-33-6(32)7(15,16)8(17,18)9(19,20)10(21,22)11(23,24
InchiKey: IPDHNBLBHIACOC-UHFFFAOYSA-N
Formula: C14H11F17O2
SMILES: CCCCCOC(=O)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 534.21

Physical Properties

Property code	Value	Unit	Source
gf	-3455.97	kJ/mol	Joback Method
hf	-3980.96	kJ/mol	Joback Method
hfus	27.85	kJ/mol	Joback Method
hvap	31.66	kJ/mol	Joback Method
log10ws	-7.41		Crippen Method
logp	6.729		Crippen Method
mcvol	245.650	ml/mol	McGowan Method
pc	1021.38	kPa	Joback Method
rinpol	1076.00		NIST Webbook
rinpol	1076.00		NIST Webbook
tb	557.76	K	Joback Method
tc	690.60	K	Joback Method
tf	349.09	K	Joback Method
vc	1.062	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	725.82	J/mol×K	557.76	Joback Method
cpg	739.47	J/mol×K	579.90	Joback Method
cpg	752.21	J/mol×K	602.04	Joback Method
cpg	764.08	J/mol×K	624.18	Joback Method
cpg	775.13	J/mol×K	646.32	Joback Method
cpg	785.41	J/mol×K	668.46	Joback Method
cpg	794.98	J/mol×K	690.60	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U356020&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

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