Heptadecafluorononanoic acid, isohexyl ester

Inchi: InChI=1S/C15H13F17O2/c1-6(2)4-3-5-34-7(33)8(16,17)9(18,19)10(20,21)11(22,23)12(24
InchiKey: LSPPKAMVPYAKFJ-UHFFFAOYSA-N
Formula: C15H13F17O2
SMILES: CC(C)CCCOC(=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]: 548.24

Physical Properties

Property code	Value	Unit	Source
gf	-3449.99	kJ/mol	Joback Method
hf	-4006.88	kJ/mol	Joback Method
hfus	26.92	kJ/mol	Joback Method
hvap	33.50	kJ/mol	Joback Method
log10ws	-7.58		Crippen Method
logp	6.975		Crippen Method
mcvol	259.740	ml/mol	McGowan Method
pc	966.27	kPa	Joback Method
rinpol	1129.00		NIST Webbook
rinpol	1129.00		NIST Webbook
tb	580.20	K	Joback Method
tc	716.53	K	Joback Method
tf	345.36	K	Joback Method
vc	1.111	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	778.45	J/mol×K	580.20	Joback Method
cpg	792.51	J/mol×K	602.92	Joback Method
cpg	805.63	J/mol×K	625.64	Joback Method
cpg	817.85	J/mol×K	648.37	Joback Method
cpg	829.23	J/mol×K	671.09	Joback Method
cpg	839.82	J/mol×K	693.81	Joback Method
cpg	849.68	J/mol×K	716.53	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U356021&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