Pentadecafluorooctanoic acid, hexyl ester

Inchi: InChI=1S/C14H13F15O2/c1-2-3-4-5-6-31-7(30)8(15,16)9(17,18)10(19,20)11(21,22)12(23
InchiKey: KHELVFSKTOQOCW-UHFFFAOYSA-N
Formula: C14H13F15O2
SMILES: CCCCCCOC(=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)F
Mol. weight [g/mol]: 498.23

Physical Properties

Property code	Value	Unit	Source
gf	-3069.19	kJ/mol	Joback Method
hf	-3579.99	kJ/mol	Joback Method
hfus	29.11	kJ/mol	Joback Method
hvap	34.59	kJ/mol	Joback Method
log10ws	-7.09		Crippen Method
logp	6.484		Crippen Method
mcvol	242.110	ml/mol	McGowan Method
pc	1069.36	kPa	Joback Method
rinpol	1116.00		NIST Webbook
rinpol	1116.00		NIST Webbook
tb	562.45	K	Joback Method
tc	698.15	K	Joback Method
tf	345.49	K	Joback Method
vc	1.036	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	706.99	J/mol×K	562.45	Joback Method
cpg	720.80	J/mol×K	585.07	Joback Method
cpg	733.72	J/mol×K	607.68	Joback Method
cpg	745.81	J/mol×K	630.30	Joback Method
cpg	757.11	J/mol×K	652.91	Joback Method
cpg	767.66	J/mol×K	675.53	Joback Method
cpg	777.52	J/mol×K	698.15	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U406036&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