Pentadecafluorooctanoic acid, heptyl ester

Inchi: InChI=1S/C15H15F15O2/c1-2-3-4-5-6-7-32-8(31)9(16,17)10(18,19)11(20,21)12(22,23)13
InchiKey: SFLCAVLNVVENEX-UHFFFAOYSA-N
Formula: C15H15F15O2
SMILES: CCCCCCCOC(=O)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]: 512.25

Physical Properties

Property code	Value	Unit	Source
gf	-3060.77	kJ/mol	Joback Method
hf	-3600.63	kJ/mol	Joback Method
hfus	31.70	kJ/mol	Joback Method
hvap	36.81	kJ/mol	Joback Method
log10ws	-7.51		Crippen Method
logp	6.874		Crippen Method
mcvol	256.200	ml/mol	McGowan Method
pc	1005.26	kPa	Joback Method
rinpol	1204.00		NIST Webbook
tb	585.33	K	Joback Method
tc	723.28	K	Joback Method
tf	356.76	K	Joback Method
vc	1.093	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	759.40	J/mol×K	585.33	Joback Method
cpg	773.51	J/mol×K	608.32	Joback Method
cpg	786.71	J/mol×K	631.31	Joback Method
cpg	799.07	J/mol×K	654.30	Joback Method
cpg	810.63	J/mol×K	677.30	Joback Method
cpg	821.44	J/mol×K	700.29	Joback Method
cpg	831.56	J/mol×K	723.28	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U406037&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