Heptadecafluorononanoic acid, ethyl ester

Inchi: InChI=1S/C11H5F17O2/c1-2-30-3(29)4(12,13)5(14,15)6(16,17)7(18,19)8(20,21)9(22,23)
InchiKey: DRLDSHOYANTUND-UHFFFAOYSA-N
Formula: C11H5F17O2
SMILES: CCOC(=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]: 492.13

Physical Properties

Property code	Value	Unit	Source
gf	-3481.23	kJ/mol	Joback Method
hf	-3919.04	kJ/mol	Joback Method
hfus	20.08	kJ/mol	Joback Method
hvap	24.98	kJ/mol	Joback Method
log10ws	-6.15		Crippen Method
logp	5.559		Crippen Method
mcvol	203.380	ml/mol	McGowan Method
pc	1238.96	kPa	Joback Method
rinpol	835.00		NIST Webbook
tb	489.12	K	Joback Method
tc	616.35	K	Joback Method
tf	315.28	K	Joback Method
vc	0.893	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	575.31	J/mol×K	489.12	Joback Method
cpg	588.28	J/mol×K	510.32	Joback Method
cpg	600.37	J/mol×K	531.53	Joback Method
cpg	611.61	J/mol×K	552.73	Joback Method
cpg	622.05	J/mol×K	573.94	Joback Method
cpg	631.73	J/mol×K	595.14	Joback Method
cpg	640.68	J/mol×K	616.35	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U356016&Units=SI

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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