Heptadecafluorononanoic acid, octyl ester

Inchi:	InChI=1S/C17H17F17O2/c1-2-3-4-5-6-7-8-36-9(35)10(18,19)11(20,21)12(22,23)13(24,25
InchiKey:	MVFZHZANFQYMQM-UHFFFAOYSA-N
Formula:	C17H17F17O2
SMILES:	CCCCCCCCOC(=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]:	576.29

Physical Properties

Property code	Value	Unit	Source
gf	-3430.71	kJ/mol	Joback Method
hf	-4042.88	kJ/mol	Joback Method
hfus	35.62	kJ/mol	Joback Method
hvap	38.34	kJ/mol	Joback Method
log10ws	-8.66		Crippen Method
logp	7.900		Crippen Method
mcvol	287.920	ml/mol	McGowan Method
pc	856.47	kPa	Joback Method
rinpol	1328.00		NIST Webbook
rinpol	1328.00		NIST Webbook
tb	626.40	K	Joback Method
tc	768.32	K	Joback Method
tf	382.90	K	Joback Method
vc	1.230	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	885.76	J/mol×K	626.40	Joback Method
cpg	900.30	J/mol×K	650.05	Joback Method
cpg	913.87	J/mol×K	673.71	Joback Method
cpg	926.52	J/mol×K	697.36	Joback Method
cpg	938.34	J/mol×K	721.01	Joback Method
cpg	949.37	J/mol×K	744.67	Joback Method
cpg	959.68	J/mol×K	768.32	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=U356024&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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