Pentadecafluorooctanoic acid, octyl ester

Inchi: InChI=1S/C16H17F15O2/c1-2-3-4-5-6-7-8-33-9(32)10(17,18)11(19,20)12(21,22)13(23,24
InchiKey: VEBKXAIAEQLIIR-UHFFFAOYSA-N
Formula: C16H17F15O2
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]: 526.28

Physical Properties

Property code	Value	Unit	Source
gf	-3052.35	kJ/mol	Joback Method
hf	-3621.27	kJ/mol	Joback Method
hfus	34.28	kJ/mol	Joback Method
hvap	39.04	kJ/mol	Joback Method
log10ws	-7.93		Crippen Method
logp	7.264		Crippen Method
mcvol	270.290	ml/mol	McGowan Method
pc	946.75	kPa	Joback Method
rinpol	1289.00		NIST Webbook
rinpol	1289.00		NIST Webbook
tb	608.21	K	Joback Method
tc	748.85	K	Joback Method
tf	368.03	K	Joback Method
vc	1.149	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	812.86	J/mol×K	608.21	Joback Method
cpg	827.29	J/mol×K	631.65	Joback Method
cpg	840.80	J/mol×K	655.09	Joback Method
cpg	853.45	J/mol×K	678.53	Joback Method
cpg	865.29	J/mol×K	701.97	Joback Method
cpg	876.38	J/mol×K	725.41	Joback Method
cpg	886.77	J/mol×K	748.85	Joback Method

Sources

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=U406038&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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