Pentadecafluorooctanoic acid, 2-ethylhexyl ester

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

InchiKey: LRNRQNCWHBHJOC-UHFFFAOYSA-N

Formula: C16H17F15O2

SMILES: CCCCC(CC)COC(=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	-3054.79	kJ/mol	Joback Method
hf	-3626.55	kJ/mol	Joback Method
hfus	30.76	kJ/mol	Joback Method
hvap	38.65	kJ/mol	Joback Method
log10ws	-7.69		Crippen Method
logp	7.120		Crippen Method
mcvol	270.290	ml/mol	McGowan Method
pc	951.42	kPa	Joback Method
rinpol	1145.00		NIST Webbook
rinpol	1145.00		NIST Webbook
tb	607.77	K	Joback Method
tc	749.27	K	Joback Method
tf	353.03	K	Joback Method
vc	1.143	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	813.21	J/mol×K	607.77	Joback Method
cpg	827.77	J/mol×K	631.35	Joback Method
cpg	841.40	J/mol×K	654.94	Joback Method
cpg	854.15	J/mol×K	678.52	Joback Method
cpg	866.08	J/mol×K	702.10	Joback Method
cpg	877.25	J/mol×K	725.69	Joback Method
cpg	887.70	J/mol×K	749.27	Joback Method

Sources

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=U406809&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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