Pentadecafluorooctanoic acid, decyl ester

Inchi: InChI=1S/C18H21F15O2/c1-2-3-4-5-6-7-8-9-10-35-11(34)12(19,20)13(21,22)14(23,24)15
InchiKey: TXLCFHCFSWGLHL-UHFFFAOYSA-N
Formula: C18H21F15O2
SMILES: CCCCCCCCCCOC(=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]: 554.33

Physical Properties

Property code	Value	Unit	Source
gf	-3035.51	kJ/mol	Joback Method
hf	-3662.55	kJ/mol	Joback Method
hfus	39.46	kJ/mol	Joback Method
hvap	43.49	kJ/mol	Joback Method
log10ws	-8.77		Crippen Method
logp	8.044		Crippen Method
mcvol	298.470	ml/mol	McGowan Method
pc	844.07	kPa	Joback Method
rinpol	1468.00		NIST Webbook
rinpol	1468.00		NIST Webbook
tb	653.97	K	Joback Method
tc	801.53	K	Joback Method
tf	390.57	K	Joback Method
vc	1.260	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	922.74	J/mol×K	653.97	Joback Method
cpg	937.92	J/mol×K	678.56	Joback Method
cpg	952.14	J/mol×K	703.16	Joback Method
cpg	965.45	J/mol×K	727.75	Joback Method
cpg	977.94	J/mol×K	752.34	Joback Method
cpg	989.66	J/mol×K	776.94	Joback Method
cpg	1000.68	J/mol×K	801.53	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=U406040&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