Heptadecafluorononanoic acid, tridecyl ester

Inchi: InChI=1S/C22H27F17O2/c1-2-3-4-5-6-7-8-9-10-11-12-13-41-14(40)15(23,24)16(25,26)1
InchiKey: VNZWTUSLODRFTP-UHFFFAOYSA-N
Formula: C22H27F17O2
SMILES: CCCCCCCCCCCCCOC(=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)C(F)(F)F
Mol. weight [g/mol]: 646.42

Physical Properties

Property code	Value	Unit	Source
gf	-3388.61	kJ/mol	Joback Method
hf	-4146.08	kJ/mol	Joback Method
hfus	48.57	kJ/mol	Joback Method
hvap	49.47	kJ/mol	Joback Method
log10ws	-10.75		Crippen Method
logp	9.850		Crippen Method
mcvol	358.370	ml/mol	McGowan Method
pc	658.47	kPa	Joback Method
rinpol	1743.00		NIST Webbook
tb	740.80	K	Joback Method
tc	910.38	K	Joback Method
tf	439.25	K	Joback Method
vc	1.510	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1169.87	J/mol×K	740.80	Joback Method
cpg	1186.94	J/mol×K	769.06	Joback Method
cpg	1202.86	J/mol×K	797.33	Joback Method
cpg	1217.75	J/mol×K	825.59	Joback Method
cpg	1231.73	J/mol×K	853.85	Joback Method
cpg	1244.90	J/mol×K	882.12	Joback Method
cpg	1257.39	J/mol×K	910.38	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=U356029&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