Heptadecafluorononanoic acid, octadecyl ester

Inchi: InChI=1S/C27H37F17O2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-46-19(45)20(2

InchiKey: JLIIHGXVUCRQOQ-UHFFFAOYSA-N

Formula: C27H37F17O2

SMILES: CCCCCCCCCCCCCCCCCCOC(=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

Mol. weight [g/mol]: 716.55

Physical Properties

Property code	Value	Unit	Source
gf	-3346.51	kJ/mol	Joback Method
hf	-4249.28	kJ/mol	Joback Method
hfus	61.52	kJ/mol	Joback Method
hvap	60.59	kJ/mol	Joback Method
log10ws	-12.85		Crippen Method
logp	11.801		Crippen Method
mcvol	428.820	ml/mol	McGowan Method
pc	521.97	kPa	Joback Method
rinpol	2193.00		NIST Webbook
tb	855.20	K	Joback Method
tc	1076.66	K	Joback Method
tf	495.60	K	Joback Method
vc	1.790	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1472.33	J/mol×K	855.20	Joback Method
cpg	1494.37	J/mol×K	892.11	Joback Method
cpg	1515.00	J/mol×K	929.02	Joback Method
cpg	1534.50	J/mol×K	965.93	Joback Method
cpg	1553.16	J/mol×K	1002.84	Joback Method
cpg	1571.24	J/mol×K	1039.75	Joback Method
cpg	1589.02	J/mol×K	1076.66	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U356034&Units=SI
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

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