Pentadecafluorooctanoic acid, isopropyl ester

Inchi: InChI=1S/C11H7F15O2/c1-3(2)28-4(27)5(12,13)6(14,15)7(16,17)8(18,19)9(20,21)10(22,
InchiKey: JTOFYIFKZCPBPA-UHFFFAOYSA-N
Formula: C11H7F15O2
SMILES: CC(C)OC(=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]: 456.15

Physical Properties

Property code	Value	Unit	Source
gf	-3096.89	kJ/mol	Joback Method
hf	-3523.35	kJ/mol	Joback Method
hfus	17.81	kJ/mol	Joback Method
hvap	27.52	kJ/mol	Joback Method
log10ws	-5.95		Crippen Method
logp	5.312		Crippen Method
mcvol	199.840	ml/mol	McGowan Method
pc	1310.85	kPa	Joback Method
rinpol	876.00		NIST Webbook
rinpol	876.00		NIST Webbook
tb	493.37	K	Joback Method
tc	626.10	K	Joback Method
tf	296.68	K	Joback Method
vc	0.863	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	556.79	J/mol×K	493.37	Joback Method
cpg	570.02	J/mol×K	515.49	Joback Method
cpg	582.37	J/mol×K	537.61	Joback Method
cpg	593.88	J/mol×K	559.73	Joback Method
cpg	604.59	J/mol×K	581.86	Joback Method
cpg	614.54	J/mol×K	603.98	Joback Method
cpg	623.78	J/mol×K	626.10	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=U406030&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