Pentadecafluorooctanoic acid, propyl ester

Inchi: InChI=1S/C11H7F15O2/c1-2-3-28-4(27)5(12,13)6(14,15)7(16,17)8(18,19)9(20,21)10(22,
InchiKey: NLRDSVJADSYYGV-UHFFFAOYSA-N
Formula: C11H7F15O2
SMILES: CCCOC(=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	-3094.45	kJ/mol	Joback Method
hf	-3518.07	kJ/mol	Joback Method
hfus	21.34	kJ/mol	Joback Method
hvap	27.91	kJ/mol	Joback Method
log10ws	-5.84		Crippen Method
logp	5.314		Crippen Method
mcvol	199.840	ml/mol	McGowan Method
pc	1303.29	kPa	Joback Method
rinpol	905.00		NIST Webbook
rinpol	905.00		NIST Webbook
tb	493.81	K	Joback Method
tc	624.73	K	Joback Method
tf	311.68	K	Joback Method
vc	0.869	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	556.66	J/mol×K	493.81	Joback Method
cpg	569.65	J/mol×K	515.63	Joback Method
cpg	581.79	J/mol×K	537.45	Joback Method
cpg	593.11	J/mol×K	559.27	Joback Method
cpg	603.65	J/mol×K	581.09	Joback Method
cpg	613.47	J/mol×K	602.91	Joback Method
cpg	622.58	J/mol×K	624.73	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=U406031&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