Pentadecafluorooctanoic acid, pent-2-yl ester

Inchi: InChI=1S/C13H11F15O2/c1-3-4-5(2)30-6(29)7(14,15)8(16,17)9(18,19)10(20,21)11(22,23
InchiKey: OKDHCKXQNFQLIZ-UHFFFAOYSA-N
Formula: C13H11F15O2
SMILES: CCCC(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]: 484.20

Physical Properties

Property code	Value	Unit	Source
gf	-3080.05	kJ/mol	Joback Method
hf	-3564.63	kJ/mol	Joback Method
hfus	22.99	kJ/mol	Joback Method
hvap	31.97	kJ/mol	Joback Method
log10ws	-6.78		Crippen Method
logp	6.092		Crippen Method
mcvol	228.020	ml/mol	McGowan Method
pc	1145.99	kPa	Joback Method
rinpol	984.00		NIST Webbook
rinpol	984.00		NIST Webbook
tb	539.13	K	Joback Method
tc	674.41	K	Joback Method
tf	319.22	K	Joback Method
vc	0.975	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	655.91	J/mol×K	539.13	Joback Method
cpg	669.65	J/mol×K	561.68	Joback Method
cpg	682.49	J/mol×K	584.22	Joback Method
cpg	694.47	J/mol×K	606.77	Joback Method
cpg	705.66	J/mol×K	629.32	Joback Method
cpg	716.08	J/mol×K	651.86	Joback Method
cpg	725.79	J/mol×K	674.41	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U406889&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