Pentadecafluorooctanoic acid, pentyl ester

Inchi: InChI=1S/C13H11F15O2/c1-2-3-4-5-30-6(29)7(14,15)8(16,17)9(18,19)10(20,21)11(22,23
InchiKey: GVXBDIIUSCUEGI-UHFFFAOYSA-N
Formula: C13H11F15O2
SMILES: CCCCCOC(=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	-3077.61	kJ/mol	Joback Method
hf	-3559.35	kJ/mol	Joback Method
hfus	26.52	kJ/mol	Joback Method
hvap	32.36	kJ/mol	Joback Method
log10ws	-6.67		Crippen Method
logp	6.094		Crippen Method
mcvol	228.020	ml/mol	McGowan Method
pc	1139.80	kPa	Joback Method
rinpol	1015.00		NIST Webbook
rinpol	1015.00		NIST Webbook
tb	539.57	K	Joback Method
tc	673.38	K	Joback Method
tf	334.22	K	Joback Method
vc	0.981	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	655.68	J/mol×K	539.57	Joback Method
cpg	669.22	J/mol×K	561.87	Joback Method
cpg	681.87	J/mol×K	584.17	Joback Method
cpg	693.70	J/mol×K	606.48	Joback Method
cpg	704.75	J/mol×K	628.78	Joback Method
cpg	715.05	J/mol×K	651.08	Joback Method
cpg	724.66	J/mol×K	673.38	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U406034&Units=SI

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