Nonanoic acid, pentafluorophenyl ester

Inchi: InChI=1S/C15H17F5O2/c1-2-3-4-5-6-7-8-9(21)22-15-13(19)11(17)10(16)12(18)14(15)20
InchiKey: NYEKCHUHJSWPKW-UHFFFAOYSA-N
Formula: C15H17F5O2
SMILES: CCCCCCCCC(=O)Oc1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]: 324.29

Physical Properties

Property code	Value	Unit	Source
gf	-1068.29	kJ/mol	Joback Method
hf	-1399.10	kJ/mol	Joback Method
hfus	44.89	kJ/mol	Joback Method
hvap	59.64	kJ/mol	Joback Method
log10ws	-6.37		Crippen Method
logp	5.038		Crippen Method
mcvol	214.740	ml/mol	McGowan Method
pc	1501.15	kPa	Joback Method
rinpol	1606.00		NIST Webbook
rinpol	1606.00		NIST Webbook
tb	666.82	K	Joback Method
tc	836.45	K	Joback Method
tf	422.94	K	Joback Method
vc	0.881	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	584.22	J/mol×K	666.82	Joback Method
cpg	597.38	J/mol×K	695.09	Joback Method
cpg	609.94	J/mol×K	723.36	Joback Method
cpg	621.91	J/mol×K	751.63	Joback Method
cpg	633.29	J/mol×K	779.90	Joback Method
cpg	644.10	J/mol×K	808.18	Joback Method
cpg	654.32	J/mol×K	836.45	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=U360665&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