Dodecanoic acid, pentafluorophenyl ester

Inchi: InChI=1S/C18H23F5O2/c1-2-3-4-5-6-7-8-9-10-11-12(24)25-18-16(22)14(20)13(19)15(21
InchiKey: QQSJYXOHBRYWNP-UHFFFAOYSA-N
Formula: C18H23F5O2
SMILES: CCCCCCCCCCCC(=O)Oc1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]: 366.37

Physical Properties

Property code	Value	Unit	Source
gf	-1043.03	kJ/mol	Joback Method
hf	-1461.02	kJ/mol	Joback Method
hfus	52.66	kJ/mol	Joback Method
hvap	66.32	kJ/mol	Joback Method
log10ws	-7.63		Crippen Method
logp	6.208		Crippen Method
mcvol	257.010	ml/mol	McGowan Method
pc	1214.90	kPa	Joback Method
rinpol	1909.00		NIST Webbook
rinpol	1909.00		NIST Webbook
tb	735.46	K	Joback Method
tc	908.12	K	Joback Method
tf	456.75	K	Joback Method
vc	1.050	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	747.94	J/mol×K	735.46	Joback Method
cpg	762.76	J/mol×K	764.24	Joback Method
cpg	776.83	J/mol×K	793.01	Joback Method
cpg	790.17	J/mol×K	821.79	Joback Method
cpg	802.80	J/mol×K	850.57	Joback Method
cpg	814.71	J/mol×K	879.35	Joback Method
cpg	825.91	J/mol×K	908.12	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U360541&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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