(Z)-3-hexenyl pentaflurobenzoate

Inchi: InChI=1S/C13H11F5O2/c1-2-3-4-5-6-20-13(19)7-8(14)10(16)12(18)11(17)9(7)15/h3-4H,2
InchiKey: XRWDLDUDVMKQGG-ARJAWSKDSA-N
Formula: C13H11F5O2
SMILES: CCC=CCCOC(=O)c1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]: 294.22

Physical Properties

Property code	Value	Unit	Source
gf	-1004.91	kJ/mol	Joback Method
hf	-1240.60	kJ/mol	Joback Method
hfus	39.91	kJ/mol	Joback Method
hvap	55.15	kJ/mol	Joback Method
log10ws	-5.32		Crippen Method
logp	3.895		Crippen Method
mcvol	182.260	ml/mol	McGowan Method
pc	1830.98	kPa	Joback Method
rinpol	1404.00		NIST Webbook
rinpol	1413.00		NIST Webbook
rinpol	1408.00		NIST Webbook
rinpol	1408.00		NIST Webbook
rinpol	1414.00		NIST Webbook
ripol	1743.00		NIST Webbook
ripol	1747.00		NIST Webbook
ripol	1746.00		NIST Webbook
ripol	1753.00		NIST Webbook
ripol	1753.00		NIST Webbook
tb	625.22	K	Joback Method
tc	800.76	K	Joback Method
tf	395.32	K	Joback Method
vc	0.750	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	460.65	J/mol×K	625.22	Joback Method
cpg	471.98	J/mol×K	654.48	Joback Method
cpg	482.79	J/mol×K	683.73	Joback Method
cpg	493.09	J/mol×K	712.99	Joback Method
cpg	502.88	J/mol×K	742.25	Joback Method
cpg	512.17	J/mol×K	771.50	Joback Method
cpg	520.97	J/mol×K	800.76	Joback Method

Sources

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=R311910&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume