Isovaleric acid, pentafluorophenyl ester

Inchi: InChI=1S/C11H9F5O2/c1-4(2)3-5(17)18-11-9(15)7(13)6(12)8(14)10(11)16/h4H,3H2,1-2H
InchiKey: WWEZUPWFTNXRAY-UHFFFAOYSA-N
Formula: C11H9F5O2
SMILES: CC(C)CC(=O)Oc1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]: 268.18

Physical Properties

Property code	Value	Unit	Source
gf	-1104.41	kJ/mol	Joback Method
hf	-1321.82	kJ/mol	Joback Method
hfus	31.01	kJ/mol	Joback Method
hvap	50.35	kJ/mol	Joback Method
log10ws	-4.46		Crippen Method
logp	3.334		Crippen Method
mcvol	158.380	ml/mol	McGowan Method
pc	2086.93	kPa	Joback Method
rinpol	1147.00		NIST Webbook
tb	574.86	K	Joback Method
tc	749.37	K	Joback Method
tf	362.86	K	Joback Method
vc	0.651	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	385.86	J/mol×K	574.86	Joback Method
cpg	396.43	J/mol×K	603.95	Joback Method
cpg	406.57	J/mol×K	633.03	Joback Method
cpg	416.27	J/mol×K	662.12	Joback Method
cpg	425.54	J/mol×K	691.20	Joback Method
cpg	434.37	J/mol×K	720.29	Joback Method
cpg	442.76	J/mol×K	749.37	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U360651&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