2-Ethylbutyric acid, pentafluorophenyl ester

Inchi: InChI=1S/C12H11F5O2/c1-3-5(4-2)12(18)19-11-9(16)7(14)6(13)8(15)10(11)17/h5H,3-4H
InchiKey: KSUBCWUYTDAQEG-UHFFFAOYSA-N
Formula: C12H11F5O2
SMILES: CCC(CC)C(=O)Oc1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]: 282.21

Physical Properties

Property code	Value	Unit	Source
gf	-1095.99	kJ/mol	Joback Method
hf	-1342.46	kJ/mol	Joback Method
hfus	33.60	kJ/mol	Joback Method
hvap	52.58	kJ/mol	Joback Method
log10ws	-4.88		Crippen Method
logp	3.724		Crippen Method
mcvol	172.470	ml/mol	McGowan Method
pc	1915.26	kPa	Joback Method
rinpol	1219.00		NIST Webbook
rinpol	1219.00		NIST Webbook
tb	597.74	K	Joback Method
tc	771.09	K	Joback Method
tf	374.13	K	Joback Method
vc	0.708	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	433.19	J/mol×K	597.74	Joback Method
cpg	444.56	J/mol×K	626.63	Joback Method
cpg	455.45	J/mol×K	655.52	Joback Method
cpg	465.86	J/mol×K	684.41	Joback Method
cpg	475.78	J/mol×K	713.31	Joback Method
cpg	485.23	J/mol×K	742.20	Joback Method
cpg	494.19	J/mol×K	771.09	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=U370228&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