2-Ethylbutyric acid, 2,3,4-trifluorophenyl ester

Inchi: InChI=1S/C12H13F3O2/c1-3-7(4-2)12(16)17-9-6-5-8(13)10(14)11(9)15/h5-7H,3-4H2,1-2
InchiKey: ISLHNHIINUYVSB-UHFFFAOYSA-N
Formula: C12H13F3O2
SMILES: CCC(CC)C(=O)Oc1ccc(F)c(F)c1F
Mol. weight [g/mol]: 246.23

Physical Properties

Property code	Value	Unit	Source
gf	-687.11	kJ/mol	Joback Method
hf	-927.30	kJ/mol	Joback Method
hfus	28.21	kJ/mol	Joback Method
hvap	52.89	kJ/mol	Joback Method
log10ws	-4.21		Crippen Method
logp	3.446		Crippen Method
mcvol	168.930	ml/mol	McGowan Method
pc	2133.46	kPa	Joback Method
rinpol	1304.00		NIST Webbook
tb	589.24	K	Joback Method
tc	775.34	K	Joback Method
tf	347.91	K	Joback Method
vc	0.671	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	417.92	J/mol×K	589.24	Joback Method
cpg	430.73	J/mol×K	620.26	Joback Method
cpg	442.93	J/mol×K	651.27	Joback Method
cpg	454.53	J/mol×K	682.29	Joback Method
cpg	465.53	J/mol×K	713.31	Joback Method
cpg	475.94	J/mol×K	744.33	Joback Method
cpg	485.77	J/mol×K	775.34	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=U370706&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume