Acetic acid, (2,3,4,5-tetrafluorophenyl)methyl ester

Inchi: InChI=1S/C9H6F4O2/c1-4(14)15-3-5-2-6(10)8(12)9(13)7(5)11/h2H,3H2,1H3
InchiKey: CFNOCQKFYCWUAD-UHFFFAOYSA-N
Formula: C9H6F4O2
SMILES: CC(=O)OCc1cc(F)c(F)c(F)c1F
Mol. weight [g/mol]: 222.14

Physical Properties

Property code	Value	Unit	Source
gf	-914.37	kJ/mol	Joback Method
hf	-1067.68	kJ/mol	Joback Method
hfus	26.66	kJ/mol	Joback Method
hvap	46.44	kJ/mol	Joback Method
log10ws	-3.38		Crippen Method
logp	2.306		Crippen Method
mcvol	128.430	ml/mol	McGowan Method
pc	2643.39	kPa	Joback Method
rinpol	1142.00		NIST Webbook
tb	525.29	K	Joback Method
tc	706.43	K	Joback Method
tf	342.21	K	Joback Method
vc	0.527	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	288.47	J/mol×K	525.29	Joback Method
cpg	297.61	J/mol×K	555.48	Joback Method
cpg	306.39	J/mol×K	585.67	Joback Method
cpg	314.80	J/mol×K	615.86	Joback Method
cpg	322.85	J/mol×K	646.05	Joback Method
cpg	330.53	J/mol×K	676.24	Joback Method
cpg	337.83	J/mol×K	706.43	Joback Method

Sources

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=U368907&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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