Pentafluoropropionic acid, isobutyl ester

Inchi: InChI=1S/C7H9F5O2/c1-4(2)3-14-5(13)6(8,9)7(10,11)12/h4H,3H2,1-2H3
InchiKey: OFRPJUYFZWOIHH-UHFFFAOYSA-N
Formula: C7H9F5O2
SMILES: CC(C)COC(=O)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 220.14

Physical Properties

Property code	Value	Unit	Source
gf	-1196.67	kJ/mol	Joback Method
hf	-1435.94	kJ/mol	Joback Method
hfus	13.72	kJ/mol	Joback Method
hvap	33.27	kJ/mol	Joback Method
log10ws	-2.35		Crippen Method
logp	2.383		Crippen Method
mcvol	125.780	ml/mol	McGowan Method
pc	2443.48	kPa	Joback Method
rinpol	677.00		NIST Webbook
tb	425.30	K	Joback Method
tc	582.92	K	Joback Method
tf	233.60	K	Joback Method
vc	0.513	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	284.63	J/mol×K	425.30	Joback Method
cpg	295.72	J/mol×K	451.57	Joback Method
cpg	306.25	J/mol×K	477.84	Joback Method
cpg	316.23	J/mol×K	504.11	Joback Method
cpg	325.67	J/mol×K	530.38	Joback Method
cpg	334.61	J/mol×K	556.65	Joback Method
cpg	343.05	J/mol×K	582.92	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U355961&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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