3-Ethoxy-1-propanol, heptafluorobutyrate

Inchi: InChI=1S/C9H11F7O3/c1-2-18-4-3-5-19-6(17)7(10,11)8(12,13)9(14,15)16/h2-5H2,1H3
InchiKey: AILFOKDIDYSKCT-UHFFFAOYSA-N
Formula: C9H11F7O3
SMILES: CCOCCCOC(=O)C(F)(F)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 300.17

Physical Properties

Property code	Value	Unit	Source
gf	-1669.17	kJ/mol	Joback Method
hf	-2005.13	kJ/mol	Joback Method
hfus	22.36	kJ/mol	Joback Method
hvap	37.59	kJ/mol	Joback Method
log10ws	-2.83		Crippen Method
logp	2.789		Crippen Method
mcvol	163.370	ml/mol	McGowan Method
pc	1872.41	kPa	Joback Method
rinpol	941.00		NIST Webbook
rinpol	941.00		NIST Webbook
tb	489.23	K	Joback Method
tc	637.93	K	Joback Method
tf	296.97	K	Joback Method
vc	0.674	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	414.43	J/mol×K	489.23	Joback Method
cpg	426.36	J/mol×K	514.01	Joback Method
cpg	437.69	J/mol×K	538.80	Joback Method
cpg	448.42	J/mol×K	563.58	Joback Method
cpg	458.59	J/mol×K	588.37	Joback Method
cpg	468.21	J/mol×K	613.15	Joback Method
cpg	477.31	J/mol×K	637.93	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=U378340&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