3-Ethoxy-1-propanol, pentafluoropropionate

Inchi: InChI=1S/C8H11F5O3/c1-2-15-4-3-5-16-6(14)7(9,10)8(11,12)13/h2-5H2,1H3
InchiKey: XADOXDYRCSSODB-UHFFFAOYSA-N
Formula: C8H11F5O3
SMILES: CCOCCCOC(=O)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 250.16

Physical Properties

Property code	Value	Unit	Source
gf	-1290.81	kJ/mol	Joback Method
hf	-1583.52	kJ/mol	Joback Method
hfus	21.02	kJ/mol	Joback Method
hvap	38.29	kJ/mol	Joback Method
log10ws	-2.10		Crippen Method
logp	2.154		Crippen Method
mcvol	145.740	ml/mol	McGowan Method
pc	2175.46	kPa	Joback Method
rinpol	911.00		NIST Webbook
rinpol	911.00		NIST Webbook
tb	471.04	K	Joback Method
tc	625.43	K	Joback Method
tf	282.10	K	Joback Method
vc	0.594	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	350.88	J/mol×K	471.04	Joback Method
cpg	362.18	J/mol×K	496.77	Joback Method
cpg	372.97	J/mol×K	522.50	Joback Method
cpg	383.25	J/mol×K	548.23	Joback Method
cpg	393.04	J/mol×K	573.96	Joback Method
cpg	402.35	J/mol×K	599.69	Joback Method
cpg	411.20	J/mol×K	625.43	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U378344&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

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