1-Ethoxy-2-propanol, pentafluoropropionate

Inchi: InChI=1S/C8H11F5O3/c1-3-15-4-5(2)16-6(14)7(9,10)8(11,12)13/h5H,3-4H2,1-2H3
InchiKey: IZWRBZXOUXMCIA-UHFFFAOYSA-N
Formula: C8H11F5O3
SMILES: CCOCC(C)OC(=O)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 250.16

Physical Properties

Property code	Value	Unit	Source
gf	-1293.25	kJ/mol	Joback Method
hf	-1588.80	kJ/mol	Joback Method
hfus	17.50	kJ/mol	Joback Method
hvap	37.90	kJ/mol	Joback Method
log10ws	-2.21		Crippen Method
logp	2.152		Crippen Method
mcvol	145.740	ml/mol	McGowan Method
pc	2191.78	kPa	Joback Method
rinpol	880.00		NIST Webbook
rinpol	880.00		NIST Webbook
tb	470.60	K	Joback Method
tc	627.96	K	Joback Method
tf	267.10	K	Joback Method
vc	0.588	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	351.02	J/mol×K	470.60	Joback Method
cpg	362.61	J/mol×K	496.83	Joback Method
cpg	373.66	J/mol×K	523.05	Joback Method
cpg	384.18	J/mol×K	549.28	Joback Method
cpg	394.18	J/mol×K	575.50	Joback Method
cpg	403.68	J/mol×K	601.73	Joback Method
cpg	412.69	J/mol×K	627.96	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=U378349&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