2-Ethyl-1-butanol, heptafluorobutyrate

Inchi: InChI=1S/C10H13F7O2/c1-3-6(4-2)5-19-7(18)8(11,12)9(13,14)10(15,16)17/h6H,3-5H2,1
InchiKey: HANGFGBMFCYXQZ-UHFFFAOYSA-N
Formula: C10H13F7O2
SMILES: CCC(CC)COC(=O)C(F)(F)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 298.20

Physical Properties

Property code	Value	Unit	Source
gf	-1558.19	kJ/mol	Joback Method
hf	-1898.83	kJ/mol	Joback Method
hfus	20.24	kJ/mol	Joback Method
hvap	37.02	kJ/mol	Joback Method
log10ws	-3.92		Crippen Method
logp	3.799		Crippen Method
mcvol	171.590	ml/mol	McGowan Method
pc	1762.45	kPa	Joback Method
rinpol	886.80		NIST Webbook
rinpol	886.80		NIST Webbook
tb	489.25	K	Joback Method
tc	639.92	K	Joback Method
tf	271.01	K	Joback Method
vc	0.707	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	434.04	J/mol×K	489.25	Joback Method
cpg	447.25	J/mol×K	514.36	Joback Method
cpg	459.76	J/mol×K	539.47	Joback Method
cpg	471.59	J/mol×K	564.59	Joback Method
cpg	482.76	J/mol×K	589.70	Joback Method
cpg	493.30	J/mol×K	614.81	Joback Method
cpg	503.25	J/mol×K	639.92	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U352363&Units=SI

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