2-Pentanol, pentafluoropropionate

Inchi: InChI=1S/C8H11F5O2/c1-3-4-5(2)15-6(14)7(9,10)8(11,12)13/h5H,3-4H2,1-2H3
InchiKey: RXIGZIPJRMHDNW-UHFFFAOYSA-N
Formula: C8H11F5O2
SMILES: CCCC(C)OC(=O)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 234.16

Physical Properties

Property code	Value	Unit	Source
gf	-1188.25	kJ/mol	Joback Method
hf	-1456.58	kJ/mol	Joback Method
hfus	16.31	kJ/mol	Joback Method
hvap	35.49	kJ/mol	Joback Method
log10ws	-3.12		Crippen Method
logp	2.916		Crippen Method
mcvol	139.870	ml/mol	McGowan Method
pc	2227.09	kPa	Joback Method
rinpol	757.30		NIST Webbook
tb	448.18	K	Joback Method
tc	605.31	K	Joback Method
tf	244.87	K	Joback Method
vc	0.570	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	326.14	J/mol×K	448.18	Joback Method
cpg	338.08	J/mol×K	474.37	Joback Method
cpg	349.41	J/mol×K	500.56	Joback Method
cpg	360.17	J/mol×K	526.75	Joback Method
cpg	370.37	J/mol×K	552.94	Joback Method
cpg	380.03	J/mol×K	579.12	Joback Method
cpg	389.18	J/mol×K	605.31	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=U352313&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

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