4-Penten-2-ol, pentafluoropropionate

Inchi: InChI=1S/C8H9F5O2/c1-3-4-5(2)15-6(14)7(9,10)8(11,12)13/h3,5H,1,4H2,2H3
InchiKey: MZTFZLPGJBHCQE-UHFFFAOYSA-N
Formula: C8H9F5O2
SMILES: C=CCC(C)OC(=O)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 232.15

Physical Properties

Property code	Value	Unit	Source
gf	-1100.41	kJ/mol	Joback Method
hf	-1331.15	kJ/mol	Joback Method
hfus	15.03	kJ/mol	Joback Method
hvap	34.82	kJ/mol	Joback Method
log10ws	-2.98		Crippen Method
logp	2.692		Crippen Method
mcvol	135.570	ml/mol	McGowan Method
pc	2318.07	kPa	Joback Method
rinpol	752.70		NIST Webbook
tb	444.86	K	Joback Method
tc	604.87	K	Joback Method
tf	243.11	K	Joback Method
vc	0.550	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	309.68	J/mol×K	444.86	Joback Method
cpg	321.11	J/mol×K	471.53	Joback Method
cpg	331.92	J/mol×K	498.20	Joback Method
cpg	342.13	J/mol×K	524.86	Joback Method
cpg	351.76	J/mol×K	551.53	Joback Method
cpg	360.84	J/mol×K	578.20	Joback Method
cpg	369.40	J/mol×K	604.87	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U352317&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