4-Penten-2-ol, heptafluorobutyrate

Inchi: InChI=1S/C9H9F7O2/c1-3-4-5(2)18-6(17)7(10,11)8(12,13)9(14,15)16/h3,5H,1,4H2,2H3
InchiKey: SJUYEKPGHWNASC-UHFFFAOYSA-N
Formula: C9H9F7O2
SMILES: C=CCC(C)OC(=O)C(F)(F)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 282.16

Physical Properties

Property code	Value	Unit	Source
gf	-1478.77	kJ/mol	Joback Method
hf	-1752.76	kJ/mol	Joback Method
hfus	16.37	kJ/mol	Joback Method
hvap	34.12	kJ/mol	Joback Method
log10ws	-3.71		Crippen Method
logp	3.327		Crippen Method
mcvol	153.200	ml/mol	McGowan Method
pc	1985.89	kPa	Joback Method
rinpol	780.20		NIST Webbook
tb	463.05	K	Joback Method
tc	616.48	K	Joback Method
tf	257.98	K	Joback Method
vc	0.631	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	371.41	J/mol×K	463.05	Joback Method
cpg	383.57	J/mol×K	488.62	Joback Method
cpg	395.02	J/mol×K	514.19	Joback Method
cpg	405.78	J/mol×K	539.77	Joback Method
cpg	415.89	J/mol×K	565.34	Joback Method
cpg	425.37	J/mol×K	590.91	Joback Method
cpg	434.26	J/mol×K	616.48	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=U352316&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