5-Hexen-1-ol, pentafluoropropionate

Inchi: InChI=1S/C9H11F5O2/c1-2-3-4-5-6-16-7(15)8(10,11)9(12,13)14/h2H,1,3-6H2
InchiKey: SBKDCGOUTAEOCE-UHFFFAOYSA-N
Formula: C9H11F5O2
SMILES: C=CCCCCOC(=O)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 246.17

Physical Properties

Property code	Value	Unit	Source
gf	-1089.55	kJ/mol	Joback Method
hf	-1346.51	kJ/mol	Joback Method
hfus	21.14	kJ/mol	Joback Method
hvap	37.44	kJ/mol	Joback Method
log10ws	-3.28		Crippen Method
logp	3.083		Crippen Method
mcvol	149.660	ml/mol	McGowan Method
pc	2102.27	kPa	Joback Method
rinpol	880.20		NIST Webbook
rinpol	880.20		NIST Webbook
tb	468.18	K	Joback Method
tc	624.47	K	Joback Method
tf	269.38	K	Joback Method
vc	0.613	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	352.24	J/mol×K	468.18	Joback Method
cpg	364.14	J/mol×K	494.23	Joback Method
cpg	375.42	J/mol×K	520.28	Joback Method
cpg	386.10	J/mol×K	546.32	Joback Method
cpg	396.22	J/mol×K	572.37	Joback Method
cpg	405.78	J/mol×K	598.42	Joback Method
cpg	414.81	J/mol×K	624.47	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U352733&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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