5-Hexen-1-ol, trifluoroacetate

Inchi: InChI=1S/C8H11F3O2/c1-2-3-4-5-6-13-7(12)8(9,10)11/h2H,1,3-6H2
InchiKey: JSEHMFGRGCOJOF-UHFFFAOYSA-N
Formula: C8H11F3O2
SMILES: C=CCCCCOC(=O)C(F)(F)F
Mol. weight [g/mol]: 196.17

Physical Properties

Property code	Value	Unit	Source
gf	-711.19	kJ/mol	Joback Method
hf	-924.90	kJ/mol	Joback Method
hfus	19.81	kJ/mol	Joback Method
hvap	38.14	kJ/mol	Joback Method
log10ws	-2.55		Crippen Method
logp	2.448		Crippen Method
mcvol	132.030	ml/mol	McGowan Method
pc	2465.36	kPa	Joback Method
rinpol	857.20		NIST Webbook
tb	449.99	K	Joback Method
tc	613.13	K	Joback Method
tf	254.51	K	Joback Method
vc	0.531	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	290.56	J/mol×K	449.99	Joback Method
cpg	301.65	J/mol×K	477.18	Joback Method
cpg	312.23	J/mol×K	504.37	Joback Method
cpg	322.32	J/mol×K	531.56	Joback Method
cpg	331.93	J/mol×K	558.75	Joback Method
cpg	341.07	J/mol×K	585.94	Joback Method
cpg	349.76	J/mol×K	613.13	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U352736&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