4-Hexen-1-ol, trifluoroacetate

Inchi: InChI=1S/C8H11F3O2/c1-2-3-4-5-6-13-7(12)8(9,10)11/h2-3H,4-6H2,1H3/b3-2+
InchiKey: VGZQUSPVQQXMSU-NSCUHMNNSA-N
Formula: C8H11F3O2
SMILES: CC=CCCCOC(=O)C(F)(F)F
Mol. weight [g/mol]: 196.17

Physical Properties

Property code	Value	Unit	Source
gf	-718.81	kJ/mol	Joback Method
hf	-933.11	kJ/mol	Joback Method
hfus	21.29	kJ/mol	Joback Method
hvap	38.77	kJ/mol	Joback Method
log10ws	-2.55		Crippen Method
logp	2.448		Crippen Method
mcvol	132.030	ml/mol	McGowan Method
pc	2490.03	kPa	Joback Method
rinpol	863.50		NIST Webbook
rinpol	863.50		NIST Webbook
tb	457.47	K	Joback Method
tc	624.90	K	Joback Method
tf	251.19	K	Joback Method
vc	0.530	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	290.91	J/mol×K	457.47	Joback Method
cpg	302.21	J/mol×K	485.38	Joback Method
cpg	312.96	J/mol×K	513.28	Joback Method
cpg	323.16	J/mol×K	541.19	Joback Method
cpg	332.85	J/mol×K	569.09	Joback Method
cpg	342.04	J/mol×K	597.00	Joback Method
cpg	350.75	J/mol×K	624.90	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U352727&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