1,5-Hexadien-3-ol, trifluoroacetate

Inchi: InChI=1S/C8H9F3O2/c1-3-5-6(4-2)13-7(12)8(9,10)11/h3-4,6H,1-2,5H2
InchiKey: RGLKSAODPZXZQM-UHFFFAOYSA-N
Formula: C8H9F3O2
SMILES: C=CCC(C=C)OC(=O)C(F)(F)F
Mol. weight [g/mol]: 194.15

Physical Properties

Property code	Value	Unit	Source
gf	-625.79	kJ/mol	Joback Method
hf	-804.75	kJ/mol	Joback Method
hfus	15.01	kJ/mol	Joback Method
hvap	37.08	kJ/mol	Joback Method
log10ws	-2.52		Crippen Method
logp	2.223		Crippen Method
mcvol	127.730	ml/mol	McGowan Method
pc	2592.49	kPa	Joback Method
rinpol	771.20		NIST Webbook
tb	446.23	K	Joback Method
tc	616.01	K	Joback Method
tf	237.75	K	Joback Method
vc	0.506	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	274.33	J/mol×K	446.23	Joback Method
cpg	285.16	J/mol×K	474.53	Joback Method
cpg	295.43	J/mol×K	502.82	Joback Method
cpg	305.17	J/mol×K	531.12	Joback Method
cpg	314.39	J/mol×K	559.42	Joback Method
cpg	323.11	J/mol×K	587.71	Joback Method
cpg	331.35	J/mol×K	616.01	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=U352716&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