cis-2-Penten-1-ol, trifluoroacetate

Inchi: InChI=1S/C7H9F3O2/c1-2-3-4-5-12-6(11)7(8,9)10/h3-4H,2,5H2,1H3/b4-3-
InchiKey: WFLBOORSJHFTGI-ARJAWSKDSA-N
Formula: C7H9F3O2
SMILES: CCC=CCOC(=O)C(F)(F)F
Mol. weight [g/mol]: 182.14

Physical Properties

Property code	Value	Unit	Source
gf	-727.23	kJ/mol	Joback Method
hf	-912.47	kJ/mol	Joback Method
hfus	18.70	kJ/mol	Joback Method
hvap	36.54	kJ/mol	Joback Method
log10ws	-2.13		Crippen Method
logp	2.058		Crippen Method
mcvol	117.940	ml/mol	McGowan Method
pc	2746.90	kPa	Joback Method
rinpol	776.90		NIST Webbook
tb	434.59	K	Joback Method
tc	603.01	K	Joback Method
tf	239.92	K	Joback Method
vc	0.474	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	250.13	J/mol×K	434.59	Joback Method
cpg	260.48	J/mol×K	462.66	Joback Method
cpg	270.30	J/mol×K	490.73	Joback Method
cpg	279.62	J/mol×K	518.80	Joback Method
cpg	288.45	J/mol×K	546.87	Joback Method
cpg	296.82	J/mol×K	574.94	Joback Method
cpg	304.75	J/mol×K	603.01	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U352713&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