cis-2-Penten-1-ol, heptafluorobutyrate

Inchi: InChI=1S/C9H9F7O2/c1-2-3-4-5-18-6(17)7(10,11)8(12,13)9(14,15)16/h3-4H,2,5H2,1H3/b
InchiKey: FSEMQZHHOLDNDZ-ARJAWSKDSA-N
Formula: C9H9F7O2
SMILES: CCC=CCOC(=O)C(F)(F)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 282.16

Physical Properties

Property code	Value	Unit	Source
gf	-1483.95	kJ/mol	Joback Method
hf	-1755.69	kJ/mol	Joback Method
hfus	21.37	kJ/mol	Joback Method
hvap	35.14	kJ/mol	Joback Method
log10ws	-3.60		Crippen Method
logp	3.329		Crippen Method
mcvol	153.200	ml/mol	McGowan Method
pc	1989.43	kPa	Joback Method
rinpol	832.20		NIST Webbook
rinpol	832.20		NIST Webbook
tb	470.97	K	Joback Method
tc	625.29	K	Joback Method
tf	269.66	K	Joback Method
vc	0.636	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	372.20	J/mol×K	470.97	Joback Method
cpg	384.19	J/mol×K	496.69	Joback Method
cpg	395.46	J/mol×K	522.41	Joback Method
cpg	406.02	J/mol×K	548.13	Joback Method
cpg	415.93	J/mol×K	573.85	Joback Method
cpg	425.21	J/mol×K	599.57	Joback Method
cpg	433.90	J/mol×K	625.29	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U352709&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