Cis-3-hexen-1-ol, pentafluoropropionate

Inchi: InChI=1S/C9H11F5O2/c1-2-3-4-5-6-16-7(15)8(10,11)9(12,13)14/h3-4H,2,5-6H2,1H3
InchiKey: OVQXQNIONBVMIU-ARJAWSKDSA-N
Formula: C9H11F5O2
SMILES: CC/C=C\CCOC(=O)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 246.18

Physical Properties

Property code	Value	Unit	Source
hf	-1454.69	kJ/mol	Cheméo Relay (1.0)
hfus	22.63	kJ/mol	Joback Method
hvap	52.27	kJ/mol	Cheméo Relay (1.0)
logp	3.083		Crippen Method
mcvol	149.660	ml/mol	McGowan Method
rinpol	883.50		NIST Webbook
rinpol	883.50		NIST Webbook
tb	405.99	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	353.02	J/mol×K	475.66	Joback Method
cpg	365.07	J/mol×K	502.36	Joback Method
cpg	376.47	J/mol×K	529.06	Joback Method
cpg	387.22	J/mol×K	555.76	Joback Method
cpg	397.37	J/mol×K	582.46	Joback Method
cpg	406.94	J/mol×K	609.16	Joback Method
cpg	415.95	J/mol×K	635.86	Joback Method

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U352288&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature