trans-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/b4-
InchiKey: OVQXQNIONBVMIU-ONEGZZNKSA-N
Formula: C9H11F5O2
SMILES: CCC=CCCOC(=O)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 246.17

Physical Properties

Property code	Value	Unit	Source
gf	-1097.17	kJ/mol	Joback Method
hf	-1354.72	kJ/mol	Joback Method
hfus	22.63	kJ/mol	Joback Method
hvap	38.06	kJ/mol	Joback Method
log10ws	-3.28		Crippen Method
logp	3.083		Crippen Method
mcvol	149.660	ml/mol	McGowan Method
pc	2121.68	kPa	Joback Method
rinpol	881.80		NIST Webbook
tb	475.66	K	Joback Method
tc	635.86	K	Joback Method
tf	266.06	K	Joback Method
vc	0.612	m3/kmol	Joback Method

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

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U352309&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

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