2-Methyl-3-hexanol, pentafluoropropionate

Inchi: InChI=1S/C10H15F5O2/c1-4-5-7(6(2)3)17-8(16)9(11,12)10(13,14)15/h6-7H,4-5H2,1-3H3
InchiKey: XXYSQNWSJDONOS-UHFFFAOYSA-N
Formula: C10H15F5O2
SMILES: CCCC(OC(=O)C(F)(F)C(F)(F)F)C(C)C
Mol. weight [g/mol]: 262.22

Physical Properties

Property code	Value	Unit	Source
gf	-1173.85	kJ/mol	Joback Method
hf	-1503.14	kJ/mol	Joback Method
hfus	17.97	kJ/mol	Joback Method
hvap	39.56	kJ/mol	Joback Method
log10ws	-3.72		Crippen Method
logp	3.552		Crippen Method
mcvol	168.050	ml/mol	McGowan Method
pc	1885.44	kPa	Joback Method
rinpol	870.00		NIST Webbook
rinpol	870.00		NIST Webbook
tb	493.50	K	Joback Method
tc	652.48	K	Joback Method
tf	252.41	K	Joback Method
vc	0.675	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	415.13	J/mol×K	493.50	Joback Method
cpg	428.82	J/mol×K	520.00	Joback Method
cpg	441.84	J/mol×K	546.49	Joback Method
cpg	454.19	J/mol×K	572.99	Joback Method
cpg	465.91	J/mol×K	599.49	Joback Method
cpg	477.01	J/mol×K	625.99	Joback Method
cpg	487.52	J/mol×K	652.48	Joback Method

Sources

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=U376266&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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