2-Methyl-3-hexanol, heptafluorobutyrate

Inchi: InChI=1S/C11H15F7O2/c1-4-5-7(6(2)3)20-8(19)9(12,13)10(14,15)11(16,17)18/h6-7H,4-5
InchiKey: YLGXFNAUUDIQQJ-UHFFFAOYSA-N
Formula: C11H15F7O2
SMILES: CCCC(OC(=O)C(F)(F)C(F)(F)C(F)(F)F)C(C)C
Mol. weight [g/mol]: 312.22

Physical Properties

Property code	Value	Unit	Source
gf	-1552.21	kJ/mol	Joback Method
hf	-1924.75	kJ/mol	Joback Method
hfus	19.30	kJ/mol	Joback Method
hvap	38.85	kJ/mol	Joback Method
log10ws	-4.45		Crippen Method
logp	4.187		Crippen Method
mcvol	185.680	ml/mol	McGowan Method
pc	1639.10	kPa	Joback Method
rinpol	916.00		NIST Webbook
rinpol	916.00		NIST Webbook
tb	511.69	K	Joback Method
tc	664.78	K	Joback Method
tf	267.28	K	Joback Method
vc	0.756	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	481.38	J/mol×K	511.69	Joback Method
cpg	495.43	J/mol×K	537.20	Joback Method
cpg	508.72	J/mol×K	562.72	Joback Method
cpg	521.29	J/mol×K	588.23	Joback Method
cpg	533.16	J/mol×K	613.75	Joback Method
cpg	544.36	J/mol×K	639.26	Joback Method
cpg	554.93	J/mol×K	664.78	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=U376265&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