2,4-Dimethyl-3-pentanol, heptafluorobutyrate

Inchi: InChI=1S/C11H15F7O2/c1-5(2)7(6(3)4)20-8(19)9(12,13)10(14,15)11(16,17)18/h5-7H,1-4
InchiKey: LFQPNHZMJJVTGX-UHFFFAOYSA-N
Formula: C11H15F7O2
SMILES: CC(C)C(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	-1554.65	kJ/mol	Joback Method
hf	-1930.03	kJ/mol	Joback Method
hfus	15.78	kJ/mol	Joback Method
hvap	38.47	kJ/mol	Joback Method
log10ws	-4.21		Crippen Method
logp	4.043		Crippen Method
mcvol	185.680	ml/mol	McGowan Method
pc	1649.77	kPa	Joback Method
rinpol	918.00		NIST Webbook
rinpol	918.00		NIST Webbook
tb	511.25	K	Joback Method
tc	667.00	K	Joback Method
tf	252.28	K	Joback Method
vc	0.750	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	481.57	J/mol×K	511.25	Joback Method
cpg	495.93	J/mol×K	537.21	Joback Method
cpg	509.50	J/mol×K	563.17	Joback Method
cpg	522.31	J/mol×K	589.12	Joback Method
cpg	534.39	J/mol×K	615.08	Joback Method
cpg	545.78	J/mol×K	641.04	Joback Method
cpg	556.52	J/mol×K	667.00	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U375655&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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