3-Heptanol, heptafluorobutyrate

Inchi: InChI=1S/C11H15F7O2/c1-3-5-6-7(4-2)20-8(19)9(12,13)10(14,15)11(16,17)18/h7H,3-6H
InchiKey: FJSJBVAURZYIPW-UHFFFAOYSA-N
Formula: C11H15F7O2
SMILES: CCCCC(CC)OC(=O)C(F)(F)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 312.22

Physical Properties

Property code	Value	Unit	Source
gf	-1549.77	kJ/mol	Joback Method
hf	-1919.47	kJ/mol	Joback Method
hfus	22.83	kJ/mol	Joback Method
hvap	39.24	kJ/mol	Joback Method
log10ws	-4.69		Crippen Method
logp	4.331		Crippen Method
mcvol	185.680	ml/mol	McGowan Method
pc	1628.54	kPa	Joback Method
rinpol	947.00		NIST Webbook
rinpol	947.00		NIST Webbook
tb	512.13	K	Joback Method
tc	662.67	K	Joback Method
tf	282.28	K	Joback Method
vc	0.762	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	481.18	J/mol×K	512.13	Joback Method
cpg	494.94	J/mol×K	537.22	Joback Method
cpg	507.97	J/mol×K	562.31	Joback Method
cpg	520.30	J/mol×K	587.40	Joback Method
cpg	531.96	J/mol×K	612.49	Joback Method
cpg	542.98	J/mol×K	637.58	Joback Method
cpg	553.39	J/mol×K	662.67	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U376267&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

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