3-Heptanol, pentafluoropropionate

Inchi: InChI=1S/C10H15F5O2/c1-3-5-6-7(4-2)17-8(16)9(11,12)10(13,14)15/h7H,3-6H2,1-2H3
InchiKey: HECFNHLGZSYGPY-UHFFFAOYSA-N
Formula: C10H15F5O2
SMILES: CCCCC(CC)OC(=O)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 262.22

Physical Properties

Property code	Value	Unit	Source
gf	-1171.41	kJ/mol	Joback Method
hf	-1497.86	kJ/mol	Joback Method
hfus	21.49	kJ/mol	Joback Method
hvap	39.95	kJ/mol	Joback Method
log10ws	-3.96		Crippen Method
logp	3.696		Crippen Method
mcvol	168.050	ml/mol	McGowan Method
pc	1872.41	kPa	Joback Method
rinpol	904.00		NIST Webbook
rinpol	904.00		NIST Webbook
tb	493.94	K	Joback Method
tc	650.03	K	Joback Method
tf	267.41	K	Joback Method
vc	0.681	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	414.96	J/mol×K	493.94	Joback Method
cpg	428.34	J/mol×K	519.95	Joback Method
cpg	441.07	J/mol×K	545.97	Joback Method
cpg	453.17	J/mol×K	571.98	Joback Method
cpg	464.66	J/mol×K	598.00	Joback Method
cpg	475.56	J/mol×K	624.01	Joback Method
cpg	485.90	J/mol×K	650.03	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=U376268&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