5-Hexen-1-ol, heptafluorobutyrate

Inchi: InChI=1S/C10H11F7O2/c1-2-3-4-5-6-19-7(18)8(11,12)9(13,14)10(15,16)17/h2H,1,3-6H2
InchiKey: QNLAGUOCYODSMS-UHFFFAOYSA-N
Formula: C10H11F7O2
SMILES: C=CCCCCOC(=O)C(F)(F)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 296.18

Physical Properties

Property code	Value	Unit	Source
gf	-1467.91	kJ/mol	Joback Method
hf	-1768.12	kJ/mol	Joback Method
hfus	22.48	kJ/mol	Joback Method
hvap	36.73	kJ/mol	Joback Method
log10ws	-4.02		Crippen Method
logp	3.719		Crippen Method
mcvol	167.290	ml/mol	McGowan Method
pc	1813.86	kPa	Joback Method
rinpol	925.50		NIST Webbook
rinpol	925.50		NIST Webbook
tb	486.37	K	Joback Method
tc	636.73	K	Joback Method
tf	284.25	K	Joback Method
vc	0.694	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	415.95	J/mol×K	486.37	Joback Method
cpg	428.41	J/mol×K	511.43	Joback Method
cpg	440.18	J/mol×K	536.49	Joback Method
cpg	451.27	J/mol×K	561.55	Joback Method
cpg	461.73	J/mol×K	586.61	Joback Method
cpg	471.57	J/mol×K	611.67	Joback Method
cpg	480.83	J/mol×K	636.73	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=U352728&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