3-Methyl-1-butanol, heptafluorobutyrate

Inchi: InChI=1S/C9H11F7O2/c1-5(2)3-4-18-6(17)7(10,11)8(12,13)9(14,15)16/h5H,3-4H2,1-2H3
InchiKey: AHKCGBGVCKMGEE-UHFFFAOYSA-N
Formula: C9H11F7O2
SMILES: CC(C)CCOC(=O)C(F)(F)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 284.17

Physical Properties

Property code	Value	Unit	Source
gf	-1566.61	kJ/mol	Joback Method
hf	-1878.19	kJ/mol	Joback Method
hfus	17.65	kJ/mol	Joback Method
hvap	34.79	kJ/mol	Joback Method
log10ws	-3.50		Crippen Method
logp	3.409		Crippen Method
mcvol	157.500	ml/mol	McGowan Method
pc	1913.58	kPa	Joback Method
rinpol	803.50		NIST Webbook
rinpol	803.50		NIST Webbook
tb	466.37	K	Joback Method
tc	617.26	K	Joback Method
tf	259.74	K	Joback Method
vc	0.650	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	388.58	J/mol×K	466.37	Joback Method
cpg	401.20	J/mol×K	491.52	Joback Method
cpg	413.14	J/mol×K	516.67	Joback Method
cpg	424.41	J/mol×K	541.81	Joback Method
cpg	435.04	J/mol×K	566.96	Joback Method
cpg	445.06	J/mol×K	592.11	Joback Method
cpg	454.50	J/mol×K	617.26	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=U352323&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