3-Buten-1-ol, heptafluorobutyrate

Inchi: InChI=1S/C8H7F7O2/c1-2-3-4-17-5(16)6(9,10)7(11,12)8(13,14)15/h2H,1,3-4H2
InchiKey: ZJZGWTZMUUCZDJ-UHFFFAOYSA-N
Formula: C8H7F7O2
SMILES: C=CCCOC(=O)C(F)(F)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 268.13

Physical Properties

Property code	Value	Unit	Source
gf	-1484.75	kJ/mol	Joback Method
hf	-1726.84	kJ/mol	Joback Method
hfus	17.30	kJ/mol	Joback Method
hvap	32.28	kJ/mol	Joback Method
log10ws	-3.18		Crippen Method
logp	2.939		Crippen Method
mcvol	139.110	ml/mol	McGowan Method
pc	2151.31	kPa	Joback Method
rinpol	760.20		NIST Webbook
rinpol	760.20		NIST Webbook
tb	440.61	K	Joback Method
tc	591.39	K	Joback Method
tf	261.71	K	Joback Method
vc	0.582	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	328.46	J/mol×K	440.61	Joback Method
cpg	339.66	J/mol×K	465.74	Joback Method
cpg	350.19	J/mol×K	490.87	Joback Method
cpg	360.09	J/mol×K	516.00	Joback Method
cpg	369.38	J/mol×K	541.13	Joback Method
cpg	378.08	J/mol×K	566.26	Joback Method
cpg	386.24	J/mol×K	591.39	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U352271&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