1-Octen-3-ol, heptafluorobutyrate

Inchi: InChI=1S/C12H15F7O2/c1-3-5-6-7-8(4-2)21-9(20)10(13,14)11(15,16)12(17,18)19/h4,8H
InchiKey: QROWCCNORFAIJS-UHFFFAOYSA-N
Formula: C12H15F7O2
SMILES: C=CC(CCCCC)OC(=O)C(F)(F)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 324.24

Physical Properties

Property code	Value	Unit	Source
gf	-1453.51	kJ/mol	Joback Method
hf	-1814.68	kJ/mol	Joback Method
hfus	24.14	kJ/mol	Joback Method
hvap	40.80	kJ/mol	Joback Method
log10ws	-4.96		Crippen Method
logp	4.497		Crippen Method
mcvol	195.470	ml/mol	McGowan Method
pc	1559.81	kPa	Joback Method
rinpol	1015.60		NIST Webbook
rinpol	1015.60		NIST Webbook
tb	531.69	K	Joback Method
tc	684.32	K	Joback Method
tf	291.79	K	Joback Method
vc	0.799	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	510.49	J/mol×K	531.69	Joback Method
cpg	524.28	J/mol×K	557.13	Joback Method
cpg	537.31	J/mol×K	582.57	Joback Method
cpg	549.62	J/mol×K	608.00	Joback Method
cpg	561.23	J/mol×K	633.44	Joback Method
cpg	572.18	J/mol×K	658.88	Joback Method
cpg	582.51	J/mol×K	684.32	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=U352750&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