1-Octen-3-ol, pentafluoropropionate

Inchi: InChI=1S/C11H15F5O2/c1-3-5-6-7-8(4-2)18-9(17)10(12,13)11(14,15)16/h4,8H,2-3,5-7H2
InchiKey: QWKJNSPWLFHFQM-UHFFFAOYSA-N
Formula: C11H15F5O2
SMILES: C=CC(CCCCC)OC(=O)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 274.23

Physical Properties

Property code	Value	Unit	Source
gf	-1075.15	kJ/mol	Joback Method
hf	-1393.07	kJ/mol	Joback Method
hfus	22.80	kJ/mol	Joback Method
hvap	41.50	kJ/mol	Joback Method
log10ws	-4.23		Crippen Method
logp	3.862		Crippen Method
mcvol	177.840	ml/mol	McGowan Method
pc	1787.88	kPa	Joback Method
rinpol	970.60		NIST Webbook
tb	513.50	K	Joback Method
tc	671.60	K	Joback Method
tf	276.92	K	Joback Method
vc	0.719	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	443.27	J/mol×K	513.50	Joback Method
cpg	456.79	J/mol×K	539.85	Joback Method
cpg	469.62	J/mol×K	566.20	Joback Method
cpg	481.78	J/mol×K	592.55	Joback Method
cpg	493.30	J/mol×K	618.90	Joback Method
cpg	504.21	J/mol×K	645.25	Joback Method
cpg	514.52	J/mol×K	671.60	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U352752&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