2-Octanol, pentafluoropropionate

Inchi: InChI=1S/C11H17F5O2/c1-3-4-5-6-7-8(2)18-9(17)10(12,13)11(14,15)16/h8H,3-7H2,1-2H
InchiKey: XSSVHQACLODJSO-UHFFFAOYSA-N
Formula: C11H17F5O2
SMILES: CCCCCCC(C)OC(=O)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 276.24

Physical Properties

Property code	Value	Unit	Source
gf	-1162.99	kJ/mol	Joback Method
hf	-1518.50	kJ/mol	Joback Method
hfus	24.08	kJ/mol	Joback Method
hvap	42.17	kJ/mol	Joback Method
log10ws	-4.38		Crippen Method
logp	4.086		Crippen Method
mcvol	182.140	ml/mol	McGowan Method
pc	1726.03	kPa	Joback Method
rinpol	1008.80		NIST Webbook
rinpol	987.00		NIST Webbook
ripol	1001.00		NIST Webbook
tb	516.82	K	Joback Method
tc	672.47	K	Joback Method
tf	278.68	K	Joback Method
vc	0.738	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	462.07	J/mol×K	516.82	Joback Method
cpg	476.07	J/mol×K	542.76	Joback Method
cpg	489.39	J/mol×K	568.70	Joback Method
cpg	502.06	J/mol×K	594.65	Joback Method
cpg	514.10	J/mol×K	620.59	Joback Method
cpg	525.53	J/mol×K	646.53	Joback Method
cpg	536.38	J/mol×K	672.47	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U352372&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume