Pentafluoropropionic acid, octyl ester

Inchi: InChI=1S/C11H17F5O2/c1-2-3-4-5-6-7-8-18-9(17)10(12,13)11(14,15)16/h2-8H2,1H3
InchiKey: ZPVRQKZQZAFDCY-UHFFFAOYSA-N
Formula: C11H17F5O2
SMILES: CCCCCCCCOC(=O)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 276.24
CAS: 1867-95-4

Physical Properties

Property code	Value	Unit	Source
gf	-1160.55	kJ/mol	Joback Method
hf	-1513.22	kJ/mol	Joback Method
hfus	27.60	kJ/mol	Joback Method
hvap	42.56	kJ/mol	Joback Method
log10ws	-4.27		Crippen Method
logp	4.088		Crippen Method
mcvol	182.140	ml/mol	McGowan Method
pc	1714.61	kPa	Joback Method
rinpol	1062.00		NIST Webbook
rinpol	1071.00		NIST Webbook
rinpol	1076.60		NIST Webbook
rinpol	1078.00		NIST Webbook
ripol	1114.00		NIST Webbook
ripol	1120.00		NIST Webbook
tb	517.26	K	Joback Method
tc	670.29	K	Joback Method
tf	293.68	K	Joback Method
vc	0.744	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	461.85	J/mol×K	517.26	Joback Method
cpg	475.56	J/mol×K	542.77	Joback Method
cpg	488.62	J/mol×K	568.27	Joback Method

cpg	501.04	J/mol×K	593.78	Joback Method
cpg	512.87	J/mol×K	619.28	Joback Method
cpg	524.11	J/mol×K	644.79	Joback Method
cpg	534.79	J/mol×K	670.29	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1867954&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