Pentafluoropropionic acid, undecyl ester

Other names: Undecyl pentafluoropropionate
Inchi: InChI=1S/C14H23F5O2/c1-2-3-4-5-6-7-8-9-10-11-21-12(20)13(15,16)14(17,18)19/h2-11
InchiKey: YZILLGCYNLQMIQ-UHFFFAOYSA-N
Formula: C14H23F5O2
SMILES: CCCCCCCCCCCOC(=O)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 318.32
CAS: 959014-11-0

Physical Properties

Property code	Value	Unit	Source
gf	-1135.29	kJ/mol	Joback Method
hf	-1575.14	kJ/mol	Joback Method
hfus	35.37	kJ/mol	Joback Method
hvap	49.24	kJ/mol	Joback Method
log10ws	-5.52		Crippen Method
logp	5.258		Crippen Method
mcvol	224.410	ml/mol	McGowan Method
pc	1368.70	kPa	Joback Method
rinpol	1357.30		NIST Webbook
rinpol	1357.30		NIST Webbook
rinpol	1355.00		NIST Webbook
tb	585.90	K	Joback Method
tc	739.25	K	Joback Method
tf	327.49	K	Joback Method
vc	0.911	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	612.68	J/mol×K	585.90	Joback Method
cpg	627.99	J/mol×K	611.46	Joback Method
cpg	642.57	J/mol×K	637.02	Joback Method
cpg	656.46	J/mol×K	662.57	Joback Method
cpg	669.68	J/mol×K	688.13	Joback Method

cpg	682.27	J/mol×K	713.69	Joback Method
cpg	694.23	J/mol×K	739.25	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C959014110&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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