Pentafluoropropionic acid, hexyl ester

Other names:	Hexyl pentafluoropropionate
	Hexyl 2,2,3,3,3-pentafluoropropanoate
	1-Hexanol, pentafluoropropionate
	2,2,3,3,3-Pentafluoro-propionic acid hexyl ester
	Hexyl pentafluoropropanoate
	Propanoic acid, pentafluoro, hexyl ester
Inchi:	InChI=1S/C9H13F5O2/c1-2-3-4-5-6-16-7(15)8(10,11)9(12,13)14/h2-6H2,1H3
InchiKey:	ZNCCRAMYHTXLQS-UHFFFAOYSA-N
Formula:	C9H13F5O2
SMILES:	CCCCCCOC(=O)C(F)(F)C(F)(F)F
Mol. weight [g/mol]:	248.19
CAS:	134639-01-3

Physical Properties

Property code	Value	Unit	Source
gf	-1177.39	kJ/mol	Joback Method
hf	-1471.94	kJ/mol	Joback Method
hfus	22.42	kJ/mol	Joback Method
hvap	38.11	kJ/mol	Joback Method
log10ws	-3.43		Crippen Method
logp	3.307		Crippen Method
mcvol	153.960	ml/mol	McGowan Method
pc	2023.58	kPa	Joback Method
rinpol	894.00		NIST Webbook
rinpol	859.00		NIST Webbook
rinpol	878.00		NIST Webbook
rinpol	894.00		NIST Webbook
rinpol	900.30		NIST Webbook
rinpol	878.00		NIST Webbook
rinpol	878.20		NIST Webbook
rinpol	882.00		NIST Webbook
ripol	907.00		NIST Webbook
ripol	919.00		NIST Webbook
tb	471.50	K	Joback Method
tc	625.16	K	Joback Method
tf	271.14	K	Joback Method
vc	0.631	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	369.49	J/mol×K	471.50	Joback Method
cpg	381.88	J/mol×K	497.11	Joback Method
cpg	393.67	J/mol×K	522.72	Joback Method
cpg	404.89	J/mol×K	548.33	Joback Method
cpg	415.54	J/mol×K	573.94	Joback Method
cpg	425.66	J/mol×K	599.55	Joback Method
cpg	435.25	J/mol×K	625.16	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C134639013&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
ripol: Polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature

tf: Normal melting (fusion) point

vc: Critical Volume