Pentafluoropropionic acid, hexadecyl ester

Other names:	Hexadecyl pentafluoropropionate
	Hexadecyl 2,2,3,3,3-pentafluoropropanoate
	1-Hexadecanol, pentafluoropropionate
	1-Hexadecanol, PFP
Inchi:	InChI=1S/C19H33F5O2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-26-17(25)18(20,21)19
InchiKey:	MKXNHVLXIYBJIK-UHFFFAOYSA-N
Formula:	C19H33F5O2
SMILES:	CCCCCCCCCCCCCCCCOC(=O)C(F)(F)C(F)(F)F
Mol. weight [g/mol]:	388.46
CAS:	6222-07-7

Physical Properties

Property code	Value	Unit	Source
gf	-1093.19	kJ/mol	Joback Method
hf	-1678.34	kJ/mol	Joback Method
hfus	48.32	kJ/mol	Joback Method
hvap	60.37	kJ/mol	Joback Method
log10ws	-7.61		Crippen Method
logp	7.209		Crippen Method
mcvol	294.860	ml/mol	McGowan Method
pc	987.02	kPa	Joback Method
rinpol	1818.00		NIST Webbook
rinpol	1817.90		NIST Webbook
rinpol	1818.00		NIST Webbook
rinpol	1817.90		NIST Webbook
rinpol	1859.00		NIST Webbook
rinpol	1859.00		NIST Webbook
ripol	1894.00		NIST Webbook
ripol	1894.00		NIST Webbook
tb	700.30	K	Joback Method
tc	861.31	K	Joback Method
tf	383.84	K	Joback Method
vc	1.192	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	890.89	J/mol×K	700.30	Joback Method
cpg	908.54	J/mol×K	727.14	Joback Method
cpg	925.33	J/mol×K	753.97	Joback Method
cpg	941.29	J/mol×K	780.81	Joback Method
cpg	956.46	J/mol×K	807.64	Joback Method
cpg	970.87	J/mol×K	834.48	Joback Method
cpg	984.57	J/mol×K	861.31	Joback Method

Sources

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=C6222077&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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