Hexadecyl pentafluoropropionate

Other names: 1-Hexadecanol, PFP
1-Hexadecanol, pentafluoropropionate
Hexadecyl 2,2,3,3,3-pentafluoropropanoate
Hexadecyl pentafluoropropionate
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

Physical Properties

Property code	Value	Unit	Source
af	0.9245		Cheméo Relay (1.0)
hf	-1753.75	kJ/mol	Cheméo Relay (1.0)
hfus	48.32	kJ/mol	Joback Method
hvap	92.22	kJ/mol	Cheméo Relay (1.0)
ie	10.55	eV	Cheméo Relay (1.0)
log10ws	-7.54		Cheméo Relay (1.0)
logp	7.209		Crippen Method
mcvol	294.860	ml/mol	McGowan Method
pc	987.02	kPa	Joback Method
tb	547.91	K	Cheméo Relay (1.0)
tc	666.45	K	Cheméo Relay (1.0)
tf	282.41	K	Cheméo Relay (1.0)
vc	1.129	m3/kmol	Cheméo Relay (1.0)

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

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C6222077&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

af: Acentric Factor
cpg: Ideal gas heat capacity
hf: Enthalpy of formation at standard conditions
hfus: Enthalpy of fusion at standard conditions
hvap: Enthalpy of vaporization at standard conditions
ie: Ionization energy
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
pc: Critical Pressure
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume