

Hexanoic acid, perfluoro-

Other names:	2,2,3,3,4,4,5,5,6,6,6-undecafluorohexanoic acid perfluoro-1-pantanecarboxylic acid perfluorohexanoic acid undecafluorohexanoic acid
Inchi:	InChI=1S/C6HF11O2/c7-2(8,1(18)19)3(9,10)4(11,12)5(13,14)6(15,16)17/h(H,18,19)
InchiKey:	PXUULQAPEKKVAH-UHFFFAOYSA-N
Formula:	C6HF11O2
SMILES:	O=C(O)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F
Mol. weight [g/mol]:	314.05
CAS:	307-24-4

Physical Properties

Property code	Value	Unit	Source
gf	-2394.81	kJ/mol	Joback Method
hf	-2632.94	kJ/mol	Joback Method
hfus	13.79	kJ/mol	Joback Method
hvap	36.91	kJ/mol	Joback Method
log10ws	-3.35		Crippen Method
logp	3.175		Crippen Method
mcvol	122.310	ml/mol	McGowan Method
pc	2405.28	kPa	Joback Method
tb	458.55	K	Joback Method
tc	595.00	K	Joback Method
tf	286.72	K	Joback Method
vc	0.539	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	373.49	J/mol×K	595.00	Joback Method
cpg	339.15	J/mol×K	481.29	Joback Method
cpg	347.24	J/mol×K	504.03	Joback Method
cpg	354.69	J/mol×K	526.78	Joback Method
cpg	361.52	J/mol×K	549.52	Joback Method

cpg	367.78	J/mol×K	572.26	Joback Method
cpg	330.37	J/mol×K	458.55	Joback Method
psub	1.26e-03	kPa	263.15	Ambient Temperature Vapor Pressure and Adsorption Capacity for (Perfluoroctyl) Ethylene, 3-(Perfluorobutyl)propanol, Perfluorohexanoic Acid, Ethyl Perfluorooctanoate, and Perfluoro-3,6-dioxaheptanoic Acid
psub	2.94e-03	kPa	270.15	Ambient Temperature Vapor Pressure and Adsorption Capacity for (Perfluoroctyl) Ethylene, 3-(Perfluorobutyl)propanol, Perfluorohexanoic Acid, Ethyl Perfluorooctanoate, and Perfluoro-3,6-dioxaheptanoic Acid
psub	7.91e-03	kPa	278.15	Ambient Temperature Vapor Pressure and Adsorption Capacity for (Perfluoroctyl) Ethylene, 3-(Perfluorobutyl)propanol, Perfluorohexanoic Acid, Ethyl Perfluorooctanoate, and Perfluoro-3,6-dioxaheptanoic Acid
psub	0.01	kPa	283.15	Ambient Temperature Vapor Pressure and Adsorption Capacity for (Perfluoroctyl) Ethylene, 3-(Perfluorobutyl)propanol, Perfluorohexanoic Acid, Ethyl Perfluorooctanoate, and Perfluoro-3,6-dioxaheptanoic Acid

psub	0.02	kPa	285.15	Ambient Temperature Vapor Pressure and Adsorption Capacity for (Perfluoroctyl) Ethylene, 3-(Perfluorobutyl)propanol, Perfluorohexanoic Acid, Ethyl Perfluorooctanoate, and Perfluoro-3,6-dioxaheptanoic Acid
psub	0.04	kPa	290.15	Ambient Temperature Vapor Pressure and Adsorption Capacity for (Perfluoroctyl) Ethylene, 3-(Perfluorobutyl)propanol, Perfluorohexanoic Acid, Ethyl Perfluorooctanoate, and Perfluoro-3,6-dioxaheptanoic Acid

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=C307244&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Ambient Temperature Vapor Pressure and Adsorption Capacity for (Perfluoroctyl) Ethylene, 3-(Perfluorobutyl)propanol, Perfluorohexanoic Acid, Ethyl Perfluorooctanoate, and Perfluoro-3,6-dioxaheptanoic Acid:	https://www.doi.org/10.1021/je400205g

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
psub:	Sublimation pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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