

Perfluoro-n-pentanoic acid

Other names:	Nonafluoro-1-pentanoic acid nonafluoropentanoic acid pentanoic acid, nonafluoro- perfluoropentanoic acid perfluorovaleric acid valeric acid, nonafluoro-
Inchi:	InChI=1S/C5HF9O2/c6-2(7,1(15)16)3(8,9)4(10,11)5(12,13)14/h(H,15,16)
InchiKey:	CXZGQIAOTKWCDDB-UHFFFAOYSA-N
Formula:	C5HF9O2
SMILES:	O=C(O)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F
Mol. weight [g/mol]:	264.05
CAS:	2706-90-3

Physical Properties

Property code	Value	Unit	Source
gf	-2016.45	kJ/mol	Joback Method
hf	-2211.33	kJ/mol	Joback Method
hfus	12.46	kJ/mol	Joback Method
hvap	37.61	kJ/mol	Joback Method
log10ws	-2.62		Crippen Method
logp	2.539		Crippen Method
mcvol	104.680	ml/mol	McGowan Method
pc	2853.57	kPa	Joback Method
tb	440.36	K	Joback Method
tc	581.40	K	Joback Method
tf	271.85	K	Joback Method
vc	0.459	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	270.53	J/mol×K	440.36	Joback Method
cpg	278.57	J/mol×K	463.87	Joback Method
cpg	285.99	J/mol×K	487.37	Joback Method

cpg	292.82	J/mol×K	510.88	Joback Method
cpg	299.10	J/mol×K	534.38	Joback Method
cpg	304.86	J/mol×K	557.89	Joback Method
cpg	310.12	J/mol×K	581.40	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Solubility of Perfluoropentanoic Acid in Supercritical Carbon Dioxide: Measurements and Modeling:	https://www.doi.org/10.1021/acs.jced.6b00649
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=C2706903&Units=SI

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

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