

2-Propanone, 1,1,1,3,3-pentafluoro-

Other names:	Pentafluoroacetone
Inchi:	InChI=1S/C3HF5O/c4-2(5)1(9)3(6,7)8/h2H
InchiKey:	WQAWXRFLNDAOON-UHFFFAOYSA-N
Formula:	C3HF5O
SMILES:	O=C(C(F)F)C(F)(F)F
Mol. weight [g/mol]:	148.03
CAS:	431-71-0

Physical Properties

Property code	Value	Unit	Source
gf	-1128.19	kJ/mol	Joback Method
hf	-1212.41	kJ/mol	Joback Method
hfus	9.59	kJ/mol	Joback Method
hvap	23.25	kJ/mol	Joback Method
log10ws	-1.33		Crippen Method
logp	1.383		Crippen Method
mcvol	63.550	ml/mol	McGowan Method
pc	3713.49	kPa	Joback Method
tb	314.59	K	Joback Method
tc	460.65	K	Joback Method
tf	163.87	K	Joback Method
vc	0.282	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	120.05	J/mol×K	314.59	Joback Method
cpg	125.93	J/mol×K	338.93	Joback Method
cpg	131.50	J/mol×K	363.28	Joback Method
cpg	136.77	J/mol×K	387.62	Joback Method
cpg	141.75	J/mol×K	411.96	Joback Method
cpg	146.45	J/mol×K	436.31	Joback Method
cpg	150.88	J/mol×K	460.65	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C431710&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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