2-Propanone, 1-fluoro-

Other names:	1-fluoro-2-propanone
	2-propanone, 1-fluoro
	CH3COCH2F
	Mono-fluoroacetone
	fluoroacetone
	propanone, fluoro-
Inchi:	InChI=1S/C3H5FO/c1-3(5)2-4/h2H2,1H3
InchiKey:	MSWVMWGCNZQPIA-UHFFFAOYSA-N
Formula:	C3H5FO
SMILES:	CC(=O)CF
Mol. weight [g/mol]:	76.07
CAS:	430-51-3

Physical Properties

Property code	Value	Unit	Source
affp	795.40	kJ/mol	NIST Webbook
basg	763.50	kJ/mol	NIST Webbook
gf	-349.35	kJ/mol	Joback Method
hf	-413.94	kJ/mol	Joback Method
hfus	8.20	kJ/mol	Joback Method
hvap	28.20	kJ/mol	Joback Method
ie	9.90	eV	NIST Webbook
ie	10.20	eV	NIST Webbook
ie	10.20 ± 0.02	eV	NIST Webbook
log10ws	-0.21		Crippen Method
logp	0.545		Crippen Method
mcvol	56.470	ml/mol	McGowan Method
pc	4516.42	kPa	Joback Method
tb	348.20	K	NIST Webbook
tc	489.24	K	Joback Method
tf	174.09	K	Joback Method
vc	0.228	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	87.73	J/mol×K	321.18	Joback Method
cpg	92.99	J/mol×K	349.19	Joback Method
cpg	98.07	J/mol×K	377.20	Joback Method
cpg	102.97	J/mol×K	405.21	Joback Method
cpg	107.70	J/mol×K	433.22	Joback Method
cpg	112.25	J/mol×K	461.23	Joback Method
cpg	116.64	J/mol×K	489.24	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Henry s Law Constants of Organic Compounds in Water and n-Octane at T = 298.2 K:	https://www.doi.org/10.1021/je900711h
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=C430513&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

affp:	Proton affinity
basg:	Gas basicity
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
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