2-Propanone, 1,3-difluoro-

Other names:	(CH2F)2CO
	1,3-Difluoroacetone
	sym-Difluoroacetone
	1,3-Difluoro-2-propanone
	1,3-Difluoropropan-2-one
	CFH2COCFH2
Inchi:	InChI=1S/C3H4F2O/c4-1-3(6)2-5/h1-2H2
InchiKey:	HKIPCXRNASWFRU-UHFFFAOYSA-N
Formula:	C3H4F2O
SMILES:	O=C(CF)CF
Mol. weight [g/mol]:	94.06
CAS:	453-14-5

Physical Properties

Property code	Value	Unit	Source
affp	762.80	kJ/mol	NIST Webbook
basg	733.00	kJ/mol	NIST Webbook
gf	-544.16	kJ/mol	Joback Method
hf	-610.05	kJ/mol	Joback Method
hfus	11.28	kJ/mol	Joback Method
hvap	27.38	kJ/mol	Joback Method
log10ws	-0.07		Crippen Method
logp	0.494		Crippen Method
mcvol	58.240	ml/mol	McGowan Method
pc	4255.16	kPa	Joback Method
tb	320.45	K	Joback Method
tc	479.02	K	Joback Method
tf	174.68	K	Joback Method
vc	0.245	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	95.95	J/mol×K	320.45	Joback Method

cpg	101.00	J/mol×K	346.88	Joback Method
cpg	105.87	J/mol×K	373.31	Joback Method
cpg	110.56	J/mol×K	399.74	Joback Method
cpg	115.09	J/mol×K	426.17	Joback Method
cpg	119.45	J/mol×K	452.59	Joback Method
cpg	123.64	J/mol×K	479.02	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C453145&Units=SI
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

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
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