2-Propanone, 1,1,1-trifluoro-

Other names:	Methyl trifluoromethyl ketone
	Trifluoromethyl methyl ketone
	1,1,1-Trifluoro-2-propanone
	1,1,1-Trifluoroacetone
	3,3,3-Trifluoroacetone
	CH3COCF3
Inchi:	InChI=1S/C3H3F3O/c1-2(7)3(4,5)6/h1H3
InchiKey:	FHUDAMLDXFJHJE-UHFFFAOYSA-N
Formula:	C3H3F3O
SMILES:	CC(=O)C(F)(F)F
Mol. weight [g/mol]:	112.05
CAS:	421-50-1

Physical Properties

Property code	Value	Unit	Source
affp	723.90	kJ/mol	NIST Webbook
basg	692.00	kJ/mol	NIST Webbook
gf	-736.13	kJ/mol	Joback Method
hf	-814.91	kJ/mol	Joback Method
hfus	6.95	kJ/mol	Joback Method
hvap	25.27	kJ/mol	Joback Method
ie	10.67 ± 0.01	eV	NIST Webbook
ie	11.00 ± 0.02	eV	NIST Webbook
log10ws	-1.02		Crippen Method
logp	1.138		Crippen Method
mcvol	60.010	ml/mol	McGowan Method
pc	4114.41	kPa	Joback Method
rinpol	459.00		NIST Webbook
tb	295.10 ± 1.00	K	NIST Webbook
tb	295.00	K	NIST Webbook
tb	295.00 ± 2.00	K	NIST Webbook
tb	294.70	K	NIST Webbook
tc	476.36	K	Joback Method
tf	177.69	K	Joback Method
vc	0.253	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	103.96	J/mol×K	316.49	Joback Method
cpg	110.11	J/mol×K	343.13	Joback Method
cpg	115.92	J/mol×K	369.78	Joback Method
cpg	121.41	J/mol×K	396.42	Joback Method
cpg	126.59	J/mol×K	423.07	Joback Method
cpg	131.48	J/mol×K	449.71	Joback Method
cpg	136.07	J/mol×K	476.36	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C421501&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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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
rinpol: Non-polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature

tf: Normal melting (fusion) point

vc: Critical Volume