

1,1,3-Trichlorotrifluoroacetone

Other names:	Acetone, 1,1,3-trichloro-1,3,3-trifluoro- 1,1,3-Trichloro-1,3,3-trifluoro-2-propanone 1,1,3-Trifluoro-1,3,3-trichloroacetone 2-Propanone, 1,1,3-trichloro-1,3,3-trifluoro- 3FK 1,1,3-Trichloro-1,3,3-trifluoroacetone
Inchi:	InChI=1S/C3Cl3F3O/c4-2(5,7)1(10)3(6,8)9
InchiKey:	QCVAFEQJWDOJLG-UHFFFAOYSA-N
Formula:	C3Cl3F3O
SMILES:	O=C(C(F)(F)Cl)C(F)(Cl)Cl
Mol. weight [g/mol]:	215.39
CAS:	79-52-7

Physical Properties

Property code	Value	Unit	Source
gf	-769.08	kJ/mol	Joback Method
hf	-870.88	kJ/mol	Joback Method
hfus	12.13	kJ/mol	Joback Method
hvap	37.13	kJ/mol	Joback Method
ie	11.21 ± 0.02	eV	NIST Webbook
log10ws	-2.58		Crippen Method
logp	2.488		Crippen Method
mvol	96.730	ml/mol	McGowan Method
pc	3668.65	kPa	Joback Method
tb	425.55	K	Joback Method
tc	623.40	K	Joback Method
tf	269.87	K	Joback Method
vc	0.389	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	168.89	J/mol×K	425.55	Joback Method
cpg	174.80	J/mol×K	458.52	Joback Method

cpg	180.07	J/mol×K	491.50	Joback Method
cpg	184.74	J/mol×K	524.47	Joback Method
cpg	188.85	J/mol×K	557.45	Joback Method
cpg	192.45	J/mol×K	590.42	Joback Method
cpg	195.59	J/mol×K	623.40	Joback Method

Sources

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=C79527&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
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

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