

Cyclobutene, hexafluoro-

Other names:	Hexafluorocyclobutene Perfluorocyclobutene 1,2,3,3,4,4-Hexafluorocyclobutene
Inchi:	InChI=1S/C4F6/c5-1-2(6)4(9,10)3(1,7)8
InchiKey:	QVHWOZCZUNPZPW-UHFFFAOYSA-N
Formula:	C4F6
SMILES:	FC1=C(F)C(F)(F)C1(F)F
Mol. weight [g/mol]:	162.03
CAS:	697-11-0

Physical Properties

Property code	Value	Unit	Source
ea	0.24	eV	NIST Webbook
gf	-1145.40	kJ/mol	Joback Method
hf	-1190.93	kJ/mol	Joback Method
hfus	9.55	kJ/mol	Joback Method
hvap	18.69	kJ/mol	Joback Method
log10ws	-2.57		Crippen Method
logp	2.421		Crippen Method
mcvol	62.680	ml/mol	McGowan Method
pc	3655.35	kPa	Joback Method
tb	278.50 ± 0.50	K	NIST Webbook
tb	278.00 ± 3.00	K	NIST Webbook
tc	449.29	K	Joback Method
tf	222.16	K	Joback Method
vc	0.297	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	115.37	J/mol×K	302.48	Joback Method
cpg	123.65	J/mol×K	326.95	Joback Method
cpg	131.11	J/mol×K	351.42	Joback Method
cpg	137.82	J/mol×K	375.88	Joback Method

cpg	143.83	J/mol×K	400.35	Joback Method
cpg	149.21	J/mol×K	424.82	Joback Method
cpg	153.99	J/mol×K	449.29	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C697110&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
ea:	Electron affinity
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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