

Cyclobutene, 4-(difluoromethylene)-2,3,3-trifluoro-1-(trifluoromethyl)

Other names:	Perfluoro(2-methyl-3-methylenecyclobutene)
Inchi:	InChI=1S/C6F8/c7-3-1(6(12,13)14)2(4(8)9)5(3,10)11
InchiKey:	IUXLZGVMGNFAJA-UHFFFAOYSA-N
Formula:	C6F8
SMILES:	FC(F)=C1C(C(F)(F)F)=C(F)C1(F)F
Mol. weight [g/mol]:	224.05
CAS:	5680-05-7

Physical Properties

Property code	Value	Unit	Source
gf	-1465.23	kJ/mol	Joback Method
hf	-1561.84	kJ/mol	Joback Method
hfus	17.72	kJ/mol	Joback Method
hvap	22.54	kJ/mol	Joback Method
log10ws	-3.96		Crippen Method
logp	3.572		Crippen Method
mcvol	90.100	ml/mol	McGowan Method
pc	2784.72	kPa	Joback Method
tb	354.50	K	Joback Method
tc	499.94	K	Joback Method
tf	225.04	K	Joback Method
vc	0.421	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	189.19	J/mol×K	354.50	Joback Method
cpg	197.53	J/mol×K	378.74	Joback Method
cpg	205.20	J/mol×K	402.98	Joback Method
cpg	212.25	J/mol×K	427.22	Joback Method
cpg	218.71	J/mol×K	451.46	Joback Method
cpg	224.64	J/mol×K	475.70	Joback Method
cpg	230.08	J/mol×K	499.94	Joback Method
hvapt	31.00	kJ/mol	274.50	NIST Webbook

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5680057&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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
h vap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
m cvol:	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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