

Butane, 1,1,3,4-tetrachloro-1,2,2,3,4,4-hexafluoro-

Other names:	Butane, 1,1,3,4-tetrachlorohexafluoro- 1,2,4,4-Tetrachloro-1,1,2,3,3,4-hexafluorobutane Hexafluoro-1,1,3,4-tetrachlorobutane 1,2,4,4-Tetrachloro-1,1,2,3,3,4-hexafluorohexane 1,1,3,4-Tetrachlorohexafluorobutane
Inchi:	InChI=1S/C4Cl4F6/c5-1(9,4(8,13)14)2(10,11)3(6,7)12
InchiKey:	CMVFABYKWZDQMC-UHFFFAOYSA-N
Formula:	C4Cl4F6
SMILES:	FC(F)(Cl)C(F)(Cl)C(F)(F)C(F)(Cl)Cl
Mol. weight [g/mol]:	303.85
CAS:	423-38-1

Physical Properties

Property code	Value	Unit	Source
gf	-1222.42	kJ/mol	Joback Method
hf	-1400.51	kJ/mol	Joback Method
hfus	11.73	kJ/mol	Joback Method
hvap	31.95	kJ/mol	Joback Method
log10ws	-4.65		Crippen Method
logp	4.459		Crippen Method
mcvol	126.800	ml/mol	McGowan Method
pc	2646.11	kPa	Joback Method
tb	406.50 ± 0.50	K	NIST Webbook
tc	607.96	K	Joback Method
tf	267.74	K	Joback Method
vc	0.519	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	246.17	J/mol×K	423.34	Joback Method
cpg	254.83	J/mol×K	454.11	Joback Method
cpg	262.50	J/mol×K	484.88	Joback Method
cpg	269.24	J/mol×K	515.65	Joback Method

cpg	275.12	J/mol×K	546.42	Joback Method
cpg	280.22	J/mol×K	577.19	Joback Method
cpg	284.60	J/mol×K	607.96	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C423381&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
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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