

2-Butyne, 1,1,1,4,4,4-hexafluoro-

Other names:	Bis(trifluoromethyl)acetylene Hexafluoro-2-butyne Perfluoro-2-butyne 1,1,1,4,4,4-Hexafluoro-2-butyne CF ₃ C «equiv» CCF ₃ Hexafluorobutyne-2 2-Butyne, hexafluoro- 1,1,1,4,4,4-hexafluorobut-2-yne
Inchi:	InChI=1S/C4F6/c5-3(6,7)1-2-4(8,9)10
InchiKey:	WBCLXFIDEDJGCC-UHFFFAOYSA-N
Formula:	C ₄ F ₆
SMILES:	FC(F)(F)C#CC(F)(F)F
Mol. weight [g/mol]:	162.03
CAS:	692-50-2

Physical Properties

Property code	Value	Unit	Source
gf	-977.58	kJ/mol	Joback Method
hf	-1047.75	kJ/mol	Joback Method
hfus	12.89	kJ/mol	Joback Method
hvap	19.16	kJ/mol	Joback Method
ie	12.35 ± 0.01	eV	NIST Webbook
ie	12.31	eV	NIST Webbook
log10ws	-2.62		Crippen Method
logp	2.114		Crippen Method
mcvol	69.240	ml/mol	McGowan Method
pc	3568.53	kPa	Joback Method
tb	248.50	K	NIST Webbook
tc	439.33	K	Joback Method
tf	249.32	K	Joback Method
vc	0.307	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	124.48	J/mol×K	289.08	Joback Method
cpg	131.52	J/mol×K	314.12	Joback Method
cpg	138.10	J/mol×K	339.16	Joback Method
cpg	144.25	J/mol×K	364.20	Joback Method
cpg	149.98	J/mol×K	389.25	Joback Method
cpg	155.32	J/mol×K	414.29	Joback Method
cpg	160.27	J/mol×K	439.33	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=C692502&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.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
hvac:	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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