

2-Butene, 2,3-dichloro-1,1,1,4,4,4-hexafluoro-

Other names:	2,3-Dichlorohexafluoro-2-butene 2,3-Dichlorohexafluorobutene-2 2-Butene, 2,3-dichlorohexafluoro- Dchfb 2,3-Dichloro-1,1,1,4,4,4-hexafluorobutene-2 trans-2,3-Dichloro-1,1,1,4,4,4-hexafluoro-2-butene 2,3-dichlorohexafluorobut-2-ene
Inchi:	InChI=1S/C4Cl2F6/c5-1(3(7,8)9)2(6)4(10,11)12/b2-1+
InchiKey:	XDIDQEGAKCWQQP-OWOJBTEDSA-N
Formula:	C4Cl2F6
SMILES:	FC(F)(F)C(Cl)=C(Cl)C(F)(F)F
Mol. weight [g/mol]:	232.94
CAS:	303-04-8

Physical Properties

Property code	Value	Unit	Source
gf	-1141.12	kJ/mol	Joback Method
hf	-1253.89	kJ/mol	Joback Method
hfus	15.74	kJ/mol	Joback Method
hvap	25.89	kJ/mol	Joback Method
ie	10.36 ± 0.01	eV	NIST Webbook
log10ws	-3.97		Crippen Method
logp	3.800		Crippen Method
mcvol	98.020	ml/mol	McGowan Method
pc	2934.52	kPa	Joback Method
tb	340.20	K	NIST Webbook
tb	341.50 ± 0.50	K	NIST Webbook
tc	521.17	K	Joback Method
tf	170.06	K	Joback Method
vc	0.425	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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cpg	179.04	J/mol×K	358.86	Joback Method
cpg	186.81	J/mol×K	385.91	Joback Method
cpg	193.95	J/mol×K	412.96	Joback Method
cpg	200.48	J/mol×K	440.01	Joback Method
cpg	206.44	J/mol×K	467.06	Joback Method
cpg	211.86	J/mol×K	494.12	Joback Method
cpg	216.77	J/mol×K	521.17	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C303048&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

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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