

1,2,4,6,6-Pentachloro-1,1,2,3,3,4,5,5,6-nonafluorohexane

Inchi:	InChI=1S/C6Cl5F9/c7-1(12,4(16,17)5(9,10)18)3(14,15)2(8,13)6(11,19)20
InchiKey:	DVAVTWADOWVBESE-UHFFFAOYSA-N
Formula:	C6Cl5F9
SMILES:	FC(F)(Cl)C(F)(Cl)C(F)(F)C(F)(Cl)C(F)(F)C(F)(Cl)Cl
Mol. weight [g/mol]:	420.31
CAS:	307-26-6

Physical Properties

Property code	Value	Unit	Source
gf	-1796.26	kJ/mol	Joback Method
hf	-2063.36	kJ/mol	Joback Method
hfus	15.52	kJ/mol	Joback Method
hvap	35.75	kJ/mol	Joback Method
log10ws	-6.41		Crippen Method
logp	5.999		Crippen Method
mcvol	172.530	ml/mol	McGowan Method
pc	1940.65	kPa	Joback Method
tb	497.88	K	Joback Method
tc	679.45	K	Joback Method
tf	326.81	K	Joback Method
vc	0.713	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	381.20	J/mol×K	497.88	Joback Method
cpg	390.53	J/mol×K	528.14	Joback Method
cpg	398.66	J/mol×K	558.40	Joback Method
cpg	405.69	J/mol×K	588.67	Joback Method
cpg	411.72	J/mol×K	618.93	Joback Method
cpg	416.85	J/mol×K	649.19	Joback Method
cpg	421.18	J/mol×K	679.45	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C307266&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

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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