

Propane, 1,1,1,3,3,3-hexafluoro-2-trifluoromethyl-

Other names:	Isobutane, perfluoro- 2-(Trifluoromethyl)-1,1,1,3,3,3-hexafluoropropane
Inchi:	InChI=1S/C4HF9/c5-2(6,7)1(3(8,9)10)4(11,12)13/h1H
InchiKey:	IMRLDNHHTCXOOR-UHFFFAOYSA-N
Formula:	C4HF9
SMILES:	FC(F)(F)C(C(F)(F)F)C(F)(F)F
Mol. weight [g/mol]:	220.04
CAS:	382-24-1

Physical Properties

Property code	Value	Unit	Source
gf	-1764.41	kJ/mol	Joback Method
hf	-1922.41	kJ/mol	Joback Method
hfus	8.07	kJ/mol	Joback Method
hvap	12.87	kJ/mol	Joback Method
log10ws	-3.24		Crippen Method
logp	3.290		Crippen Method
mvol	83.150	ml/mol	McGowan Method
pc	2651.56	kPa	Joback Method
tb	286.00 ± 1.00	K	NIST Webbook
tc	393.42	K	Joback Method
tf	132.41	K	Joback Method
vc	0.383	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	160.00	J/mol×K	274.22	Joback Method
cpg	169.10	J/mol×K	294.09	Joback Method
cpg	177.72	J/mol×K	313.95	Joback Method
cpg	185.89	J/mol×K	333.82	Joback Method
cpg	193.62	J/mol×K	353.68	Joback Method
cpg	200.93	J/mol×K	373.55	Joback Method
cpg	207.82	J/mol×K	393.42	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C382241&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
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
hvpap:	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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