

Perfluorobutyl iodide

Other names:	n-Nonafluorobutyl iodide Nonafluoro-1-iodobutane m-Nonafluorobutyl iodide Nonafluorobutyl iodide Butane, 1,1,1,2,2,3,3,4,4-nonafluoro-4-iodo- 1,1,1,2,2,3,3,4,4-nonafluoro-4-iodobutane 1-Iodononafluorobutane
Inchi:	InChI=1S/C4F9I/c5-1(6,3(9,10)11)2(7,8)4(12,13)14
InchiKey:	PGRFXXCKHGIFSV-UHFFFAOYSA-N
Formula:	C4F9I
SMILES:	FC(F)(F)C(F)(F)C(F)(F)C(F)(F)I
Mol. weight [g/mol]:	345.93
CAS:	423-39-2

Physical Properties

Property code	Value	Unit	Source
gf	-1701.01	kJ/mol	Joback Method
hf	-1849.01	kJ/mol	Joback Method
hfus	8.59	kJ/mol	Joback Method
hvap	21.33	kJ/mol	Joback Method
log10ws	-4.54		Crippen Method
logp	3.847		Crippen Method
mcvol	108.970	ml/mol	McGowan Method
pc	2621.78	kPa	Joback Method
tb	340.00	K	NIST Webbook
tc	524.56	K	Joback Method
tf	207.89	K	Joback Method
vc	0.466	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	216.72	J/mol×K	364.57	Joback Method
cpg	226.61	J/mol×K	391.23	Joback Method

cpg	235.61	J/mol×K	417.90	Joback Method
cpg	243.77	J/mol×K	444.56	Joback Method
cpg	251.14	J/mol×K	471.23	Joback Method
cpg	257.76	J/mol×K	497.89	Joback Method
cpg	263.69	J/mol×K	524.56	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=C423392&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.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
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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