Heptafluoropropyliodide

Other names:	n-Heptafluoropropyl iodide
	Heptafluoro-n-propyl iodide
	1-Iodoperfluoropropane
	Propane, 1,1,1,2,2,3,3-heptafluoro-3-iodo-
	Heptafluoro-1-iodopropane
	Heptafluoropropyl iodide
	Propane, heptafluoro-1-iodo-
	1-Iodoheptafluoropropane
	1,1,1,2,2,3,3-Heptafluoro-3-iodopropane
	1-Perfluoropropyl iodide
	Heptafluoro-1-iodo-n-propane
	1,1,2,2,3,3,3-Heptafluoro-1-iodopropane
	NSC 66409
Inchi:	InChI=1S/C3F7I/c4-1(5,2(6,7)8)3(9,10)11
InchiKey:	XTGYEAXBNRVNQU-UHFFFAOYSA-N
Formula:	C3F7I
SMILES:	FC(F)(F)C(F)(F)C(F)(F)I
Mol. weight [g/mol]:	295.92

Physical Properties

Property code	Value	Unit	Source
af	0.3085		Cheméo Relay (1.0)
gf	-1322.65	kJ/mol	Joback Method
hf	-1420.25	kJ/mol	Cheméo Relay (1.0)
hfus	7.25	kJ/mol	Joback Method
hvap	28.43	kJ/mol	Cheméo Relay (1.0)
ie	10.36 ± 0.01	eV	NIST Webbook
logp	3.212		Crippen Method
mcvol	91.340	ml/mol	McGowan Method
pc	3135.00	kPa	Joback Method
tb	314.00	K	NIST Webbook
tb	313.00	K	NIST Webbook
tc	444.13	K	Cheméo Relay (1.0)
tf	132.57	K	Cheméo Relay (1.0)
vc	0.355	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	165.12	J/mol×K	346.38	Joback Method
cpg	173.46	J/mol×K	374.30	Joback Method
cpg	181.04	J/mol×K	402.23	Joback Method
cpg	187.90	J/mol×K	430.15	Joback Method
cpg	194.06	J/mol×K	458.07	Joback Method
cpg	199.59	J/mol×K	486.00	Joback Method
cpg	204.51	J/mol×K	513.92	Joback Method

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C754347&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

af: Acentric Factor
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
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