

Heptafluoro-2-iodopropane

Other names:	Propane, heptafluoro-2-iodo- Heptafluoro-2-iodopropane Heptafluoroisopropyl iodide Isoheptafluoropropyl iodide Perfluoro-2-iodopropane Perfluoroisopropyl iodide 2-Iodoheptafluoropropane 2-Iodoperfluoropropane 1,1,1,2,3,3,3-heptafluoro-2-iodopropane
Inchi:	InChI=1S/C3F7I/c4-1(11,2(5,6)7)3(8,9)10
InchiKey:	BBZVTTKMXRPMHZ-UHFFFAOYSA-N
Formula:	C3F7I
SMILES:	FC(F)(F)C(F)(I)C(F)(F)F
Mol. weight [g/mol]:	295.92

Physical Properties

Property code	Value	Unit	Source
gf	-1322.65	kJ/mol	Joback Method
hf	-1438.67	kJ/mol	Cheméo Relay (1.0)
hfus	7.25	kJ/mol	Joback Method
ie	10.57	eV	Cheméo Relay (1.0)
logp	3.212		Crippen Method
mcvol	91.340	ml/mol	McGowan Method
pc	3135.00	kPa	Joback Method
tb	311.20	K	NIST Webbook
tb	311.00	K	NIST Webbook
tb	313.20	K	NIST Webbook
tc	457.26	K	Cheméo Relay (1.0)
tf	150.51	K	Cheméo Relay (1.0)
vc	0.351	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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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

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
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C677690&Units=SI

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
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

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