

Perfluoropropyl iodide

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]:	295.93
CAS:	754-34-7

Physical Properties

Property code	Value	Unit	Source
gf	-1322.65	kJ/mol	Joback Method
hf	-1427.40	kJ/mol	Joback Method
hfus	7.25	kJ/mol	Joback Method
hvap	22.04	kJ/mol	Joback Method
ie	10.36 ± 0.01	eV	NIST Webbook
log10ws	-3.81		Crippen Method
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	513.92	K	Joback Method
tf	193.02	K	Joback Method
vc	0.385	m3/kmol	Joback Method

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

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C754347&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
ie:	Ionization energy
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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