Perfluorooctyl iodide

Other names:	1-Iodoperfluorooctane
	Octane, 1,1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8-heptadecafluoro-8-iodo-
	1-Iodoheptadecafluorooctane
	Octane, heptadecafluoro-1-iodo-
	Heptadecafluoro-1-iodooctane
	Perfluoro-1-iodooctane
Inchi:	InChI=1S/C8F17I/c9-1(10,3(13,14)5(17,18)7(21,22)23)2(11,12)4(15,16)6(19,20)8(24,25)
InchiKey:	KWXGJTSJUKTDQU-UHFFFAOYSA-N
Formula:	C8F17I
SMILES:	FC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)I
Mol. weight [g/mol]:	545.96
CAS:	507-63-1

Physical Properties

Property code	Value	Unit	Source
gf	-3214.45	kJ/mol	Joback Method
hf	-3535.45	kJ/mol	Joback Method
hfus	13.93	kJ/mol	Joback Method
hvap	18.52	kJ/mol	Joback Method
log10ws	-7.47		Crippen Method
logp	6.388		Crippen Method
mcvol	179.490	ml/mol	McGowan Method
pc	1455.68	kPa	Joback Method
tb	433.50 ± 0.50	K	NIST Webbook
tc	573.67	K	Joback Method
tf	267.37	K	Joback Method
vc	0.789	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	450.01	J/mol×K	437.33	Joback Method
cpg	462.83	J/mol×K	460.05	Joback Method
cpg	474.56	J/mol×K	482.78	Joback Method

cpg	485.26	J/mol×K	505.50	Joback Method
cpg	494.99	J/mol×K	528.23	Joback Method
cpg	503.80	J/mol×K	550.95	Joback Method
cpg	511.75	J/mol×K	573.67	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C507631&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
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