Octane, 1,1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8-heptadecafluoro-8-i

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

Physical Properties

Property code	Value	Unit	Source
af	0.5329		Cheméo Relay (1.0)
gf	-3214.45	kJ/mol	Joback Method
hf	-3518.39	kJ/mol	Cheméo Relay (1.0)
hfus	13.93	kJ/mol	Joback Method
hvap	51.79	kJ/mol	Cheméo Relay (1.0)
ie	10.38	eV	Cheméo Relay (1.0)
logp	6.388		Crippen Method
mcvol	179.490	ml/mol	McGowan Method
pc	1455.68	kPa	Joback Method
tb	424.95	K	Cheméo Relay (1.0)
tc	563.19	K	Cheméo Relay (1.0)
tf	255.75	K	Cheméo Relay (1.0)
vc	0.771	m3/kmol	Cheméo Relay (1.0)

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
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=C507631&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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