Perfluoroheptyl iodide

Other names:	Perfluoro-n-heptyl iodide
	1-Iodoperfluoroheptane
	Heptane, 1,1,1,2,2,3,3,4,4,5,5,6,6,7,7-pentadecafluoro-7-iodo-
	1,1,1,2,2,3,3,4,4,5,5,6,6,7,7-pentadecafluoro-7-iodoheptane
Inchi:	InChI=1S/C7F15I/c8-1(9,2(10,11)4(14,15)6(18,19)20)3(12,13)5(16,17)7(21,22)23
InchiKey:	AHUMDLIBMIYQMU-UHFFFAOYSA-N
Formula:	C7F15I
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)I
Mol. weight [g/mol]:	495.96
CAS:	335-58-0

Physical Properties

Property code	Value	Unit	Source
gf	-2836.09	kJ/mol	Joback Method
hf	-3113.84	kJ/mol	Joback Method
hfus	12.59	kJ/mol	Joback Method
hvap	19.22	kJ/mol	Joback Method
log10ws	-6.74		Crippen Method
logp	5.753		Crippen Method
mcvol	161.860	ml/mol	McGowan Method
pc	1660.55	kPa	Joback Method
tb	410.50 ± 0.50	K	NIST Webbook
tc	560.34	K	Joback Method
tf	252.50	K	Joback Method
vc	0.709	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	388.21	J/mol×K	419.14	Joback Method
cpg	400.65	J/mol×K	442.67	Joback Method
cpg	412.03	J/mol×K	466.21	Joback Method
cpg	422.41	J/mol×K	489.74	Joback Method
cpg	431.83	J/mol×K	513.28	Joback Method

cpg	440.36	J/mol×K	536.81	Joback Method
cpg	448.05	J/mol×K	560.34	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C335580&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