1,8-Diiodoperfluorooctane

Inchi: InChI=1S/C8F16I2/c9-1(10,3(13,14)5(17,18)7(21,22)25)2(11,12)4(15,16)6(19,20)8(23,24
InchiKey: SRDQTCUHAMDAMG-UHFFFAOYSA-N
Formula: C8F16I2
SMILES: FC(F)(I)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]: 653.87

Physical Properties

Property code	Value	Unit	Source
gf	-2961.52	kJ/mol	Joback Method
hf	-3262.47	kJ/mol	Joback Method
hfus	15.26	kJ/mol	Joback Method
hvap	28.71	kJ/mol	Joback Method
log10ws	-8.57		Crippen Method
logp	6.854		Crippen Method
mcvol	203.540	ml/mol	McGowan Method
pc	1481.57	kPa	Joback Method
rinpol	1132.00		NIST Webbook
rinpol	1132.00		NIST Webbook
rinpol	1131.00		NIST Webbook
rinpol	1132.00		NIST Webbook
tb	531.20	K	Joback Method
tc	698.67	K	Joback Method
tf	324.84	K	Joback Method
vc	0.860	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	503.04	J/mol×K	531.20	Joback Method
cpg	513.23	J/mol×K	559.11	Joback Method
cpg	522.15	J/mol×K	587.02	Joback Method
cpg	529.89	J/mol×K	614.93	Joback Method
cpg	536.57	J/mol×K	642.84	Joback Method
cpg	542.30	J/mol×K	670.76	Joback Method

cpg	547.18	J/mol×K	698.67	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R41025&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
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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume