1,2-Diiodotetrafluoroethane

Other names: 1,1,2,2-tetrafluoro-1,2-diiodoethane
Inchi: InChI=1S/C2F4I2/c3-1(4,7)2(5,6)8
InchiKey: NZXVPCQHQVWOFD-UHFFFAOYSA-N
Formula: C2F4I2
SMILES: FC(F)(I)C(F)(F)I
Mol. weight [g/mol]: 353.82
CAS: 354-65-4

Physical Properties

Property code	Value	Unit	Source
gf	-691.36	kJ/mol	Joback Method
hf	-667.00 ± 3.00	kJ/mol	NIST Webbook
hfus	7.24	kJ/mol	Joback Method
hvap	32.93	kJ/mol	Joback Method
ie	10.11 ± 0.01	eV	NIST Webbook
log10ws	-4.17		Crippen Method
logp	3.042		Crippen Method
mcvol	97.760	ml/mol	McGowan Method
pc	3925.85	kPa	Joback Method
rinpol	790.00		NIST Webbook
rinpol	794.00		NIST Webbook
rinpol	791.00		NIST Webbook
tb	386.00 ± 2.00	K	NIST Webbook
tb	385.50 ± 0.50	K	NIST Webbook
tc	651.53	K	Joback Method
tf	235.62	K	Joback Method
vc	0.373	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	143.11	J/mol×K	422.06	Joback Method
cpg	148.54	J/mol×K	460.30	Joback Method
cpg	153.09	J/mol×K	498.55	Joback Method

cpg	156.85	J/mol×K	536.79	Joback Method
cpg	159.91	J/mol×K	575.04	Joback Method
cpg	162.35	J/mol×K	613.28	Joback Method
cpg	164.26	J/mol×K	651.53	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C354654&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume