

Pentafluoroethyl iodide

Other names:	C2F5I Perfluoroethyl iodide Iodoperfluoroethane Ethane, pentafluoroiodo- Ethane, iodopentafluoro- pentafluoroiodoethane
Inchi:	InChI=1S/C2F5I/c3-1(4,5)2(6,7)8
InchiKey:	UXPOJVLZTPGWFX-UHFFFAOYSA-N
Formula:	C2F5I
SMILES:	FC(F)(F)C(F)(F)I
Mol. weight [g/mol]:	245.92
CAS:	354-64-3

Physical Properties

Property code	Value	Unit	Source
gf	-944.29	kJ/mol	Joback Method
hf	-1005.79	kJ/mol	Joback Method
hfus	5.91	kJ/mol	Joback Method
hvap	22.74	kJ/mol	Joback Method
ie	10.70 ± 0.10	eV	NIST Webbook
ie	10.44	eV	NIST Webbook
log10ws	-3.08		Crippen Method
logp	2.576		Crippen Method
mcvol	73.710	ml/mol	McGowan Method
pc	3815.10	kPa	Joback Method
tb	285.50 ± 0.50	K	NIST Webbook
tb	285.70	K	NIST Webbook
tb	285.50 ± 0.50	K	NIST Webbook
tc	503.88	K	Joback Method
tf	178.15	K	Joback Method
vc	0.303	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	142.80	J/mol×K	474.60	Joback Method
cpg	116.77	J/mol×K	328.19	Joback Method
cpg	123.12	J/mol×K	357.47	Joback Method
cpg	128.86	J/mol×K	386.75	Joback Method
cpg	134.03	J/mol×K	416.04	Joback Method
cpg	138.67	J/mol×K	445.32	Joback Method
cpg	146.47	J/mol×K	503.88	Joback Method
hvapt	20.80	kJ/mol	265.50	NIST Webbook

Sources

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=C354643&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
hvapt:	Enthalpy of vaporization at a given temperature
ie:	Ionization energy
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

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