1,1,1-Trifluoro-2-iodoethane

Other names:	2,2,2-Trifluoroethyl iodide
	CF3CH2I
	2-Iodo-1,1,1-trifluoroethane
	Trifluoroethyl iodide
	1H,1H-Perfluoroethyl iodide
	Ethane, 1,1,1-trifluoro-2-iodo-
	1,1,1-trifluoroiodoethane
Inchi:	InChI=1S/C2H2F3I/c3-2(4,5)1-6/h1H2
InchiKey:	RKOUFQLNMRAACI-UHFFFAOYSA-N
Formula:	C2H2F3I
SMILES:	FC(F)(F)CI
Mol. weight [g/mol]:	209.94
CAS:	353-83-3

Physical Properties

Property code	Value	Unit	Source
gf	-557.51	kJ/mol	Joback Method
hf	-648.70 ± 3.90	kJ/mol	NIST Webbook
hfus	7.17	kJ/mol	Joback Method
hvap	25.67	kJ/mol	Joback Method
ie	10.00 ± 0.01	eV	NIST Webbook
ie	10.00	eV	NIST Webbook
log10ws	-2.27		Crippen Method
logp	1.984		Crippen Method
mcvol	70.170	ml/mol	McGowan Method
pc	4173.09	kPa	Joback Method
tb	327.70	K	NIST Webbook
tb	328.50 ± 0.50	K	NIST Webbook
tc	517.63	K	Joback Method
tf	174.55	K	Joback Method
vc	0.279	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	100.00	J/mol×K	332.88	Joback Method
cpg	105.40	J/mol×K	363.67	Joback Method
cpg	110.37	J/mol×K	394.46	Joback Method
cpg	114.91	J/mol×K	425.26	Joback Method
cpg	119.07	J/mol×K	456.05	Joback Method
cpg	122.85	J/mol×K	486.84	Joback Method
cpg	126.29	J/mol×K	517.63	Joback Method

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=C353833&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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
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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