1H,1H-Pentafluoropropyl iodide

Other names:	Pentafluoropropyl iodide Propane, 1,1,1,2,2-pentafluoro-3-iodo- 2,2,3,3,3-Pentafluoropropyl iodide 1,1,1,2,2-pentafluoro-3-iodopropane
Inchi:	InChI=1S/C3H2F5I/c4-2(5,1-9)3(6,7)8/h1H2
InchiKey:	HENALDZJQYAUBN-UHFFFAOYSA-N
Formula:	C3H2F5I
SMILES:	FC(F)(F)C(F)(F)CI
Mol. weight [g/mol]:	259.94
CAS:	354-69-8

Physical Properties

Property code	Value	Unit	Source
gf	-935.87	kJ/mol	Joback Method
hf	-1026.43	kJ/mol	Joback Method
hfus	8.50	kJ/mol	Joback Method
hvap	24.97	kJ/mol	Joback Method
log10ws	-3.00		Crippen Method
logp	2.619		Crippen Method
mcvol	87.800	ml/mol	McGowan Method
pc	3399.94	kPa	Joback Method
tb	351.07	K	Joback Method
tc	526.86	K	Joback Method
tf	189.42	K	Joback Method
vc	0.359	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	148.04	J/mol×K	351.07	Joback Method
cpg	155.67	J/mol×K	380.37	Joback Method
cpg	162.65	J/mol×K	409.67	Joback Method
cpg	169.02	J/mol×K	438.97	Joback Method
cpg	174.82	J/mol×K	468.27	Joback Method

cpg	180.07	J/mol×K	497.56	Joback Method
cpg	184.82	J/mol×K	526.86	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C354698&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
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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