

1,1,1-Trifluoro-3-iodobutane

Inchi:	InChI=1S/C4H6F3I/c1-3(8)2-4(5,6)7/h3H,2H2,1H3
InchiKey:	SYXQWKHNRKDCIF-UHFFFAOYSA-N
Formula:	C4H6F3I
SMILES:	CC(I)CC(F)(F)F
Mol. weight [g/mol]:	237.99
CAS:	540-87-4

Physical Properties

Property code	Value	Unit	Source
gf	-543.11	kJ/mol	Joback Method
hf	-651.38	kJ/mol	Joback Method
hfus	8.82	kJ/mol	Joback Method
hvap	29.74	kJ/mol	Joback Method
log10ws	-3.22		Crippen Method
logp	2.762		Crippen Method
mcvol	98.350	ml/mol	McGowan Method
pc	3333.53	kPa	Joback Method
tb	378.20	K	Joback Method
tc	566.53	K	Joback Method
tf	182.09	K	Joback Method
vc	0.385	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	200.94	J/molxK	535.14	Joback Method
cpg	163.64	J/molxK	378.20	Joback Method
cpg	172.21	J/molxK	409.59	Joback Method
cpg	180.19	J/molxK	440.98	Joback Method
cpg	187.63	J/molxK	472.36	Joback Method
cpg	194.53	J/molxK	503.75	Joback Method
cpg	206.89	J/molxK	566.53	Joback Method
hvapt	32.40	kJ/mol	312.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.49988e+01
Coeff. B	-3.89137e+03
Temperature range (K), min.	264.52
Temperature range (K), max.	401.70

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C540874&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature

tf: Normal melting (fusion) point

vc: Critical Volume

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