

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
hfus	8.82	kJ/mol	Joback Method
logp	2.762		Crippen Method
mcvol	98.350	ml/mol	McGowan Method
tb	381.23	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	163.64	J/mol×K	378.20	Joback Method
cpg	172.21	J/mol×K	409.59	Joback Method
cpg	180.19	J/mol×K	440.98	Joback Method
cpg	187.63	J/mol×K	472.36	Joback Method
cpg	194.53	J/mol×K	503.75	Joback Method
cpg	200.94	J/mol×K	535.14	Joback Method
cpg	206.89	J/mol×K	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

Cheméo Relay (1.0, beta):

The Yaws Handbook of Vapor Pressure:
NIST Webbook:

<https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure>

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C540874&Units=SI>

Joback Method:

https://en.wikipedia.org/wiki/Joback_method

McGowan Method:

<http://link.springer.com/article/10.1007/BF02311772>

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Crippen Method:

https://www.cheméo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature

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