

1-Propyne, 3-iodo-

Other names:	3-Iodo-1-propyne 3-Iodopropyne Propargyl iodide Propyne, 3-iodo-
Inchi:	InChI=1S/C3H3I/c1-2-3-4/h1H,3H2
InchiKey:	WGCICQJXVYFFCA-UHFFFAOYSA-N
Formula:	C3H3I
SMILES:	C#CCI
Mol. weight [g/mol]:	165.96
CAS:	659-86-9

Physical Properties

Property code	Value	Unit	Source
gf	255.57	kJ/mol	Joback Method
hf	263.52	kJ/mol	Joback Method
hfus	10.91	kJ/mol	Joback Method
hvap	31.50	kJ/mol	Joback Method
log10ws	-1.82		Crippen Method
logp	1.055		Crippen Method
mcvol	70.350	ml/mol	McGowan Method
pc	5251.00	kPa	Joback Method
tb	351.30	K	Joback Method
tc	573.63	K	Joback Method
tf	228.60	K	Joback Method
vc	0.254	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	84.64	J/molxK	351.30	Joback Method
cpg	88.63	J/molxK	388.36	Joback Method
cpg	92.29	J/molxK	425.41	Joback Method
cpg	95.64	J/molxK	462.47	Joback Method
cpg	98.71	J/molxK	499.52	Joback Method

cpg	101.53	J/mol×K	536.58	Joback Method
cpg	104.11	J/mol×K	573.63	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.45022e+01
Coeff. B	-3.36124e+03
Coeff. C	-4.90560e+01
Temperature range (K), min.	285.52
Temperature range (K), max.	414.78

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C659869&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

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
pvap:	Vapor pressure

tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume

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