

1,1-Diethylpropargylamine

Other names:	1-Pentyn-3-amine, 3-ethyl- 1,1-Diethylproparagyl amine 3-ethylpent-1-yn-3-amine
Inchi:	InChI=1S/C7H13N/c1-4-7(8,5-2)6-3/h1H,5-6,8H2,2-3H3
InchiKey:	WHNOKDNCUNZBLW-UHFFFAOYSA-N
Formula:	C7H13N
SMILES:	C#CC(N)(CC)CC
Mol. weight [g/mol]:	111.18
CAS:	3234-64-8

Physical Properties

Property code	Value	Unit	Source
gf	300.42	kJ/mol	Joback Method
hf	129.13	kJ/mol	Joback Method
hfus	14.64	kJ/mol	Joback Method
hvap	40.38	kJ/mol	Joback Method
log10ws	-2.09		Crippen Method
logp	1.137		Crippen Method
mcvol	110.870	ml/mol	McGowan Method
pc	3602.88	kPa	Joback Method
tb	418.98	K	Joback Method
tc	623.67	K	Joback Method
tf	301.30	K	Joback Method
vc	0.407	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	224.87	J/mol×K	418.98	Joback Method
cpg	237.36	J/mol×K	453.09	Joback Method
cpg	249.08	J/mol×K	487.21	Joback Method
cpg	260.07	J/mol×K	521.32	Joback Method
cpg	270.36	J/mol×K	555.44	Joback Method
cpg	280.00	J/mol×K	589.55	Joback Method

cpg

289.04

J/mol×K

623.67

Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	344.70	K	12.00	NIST Webbook

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=C3234648&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
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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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