1,1-Diethylproparagyl amine

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]: 111.19

Physical Properties

Property code	Value	Unit	Source
hfus	14.64	kJ/mol	Joback Method
ie	8.76	eV	Cheméo Relay (1.0)
logp	1.137		Crippen Method
mcvol	110.870	ml/mol	McGowan Method
tb	399.07	K	Cheméo Relay (1.0)
tf	261.54	K	Cheméo Relay (1.0)

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C3234648&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.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):

Legend

cpg: Ideal gas heat capacity
hfus: Enthalpy of fusion at standard conditions
ie: Ionization energy
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
tb: Normal Boiling Point Temperature
tbrp: Boiling point at reduced pressure
tf: Normal melting (fusion) point