

2-PENTYN-1-AMINE, N,N-DIETHYL-

Other names:	1-Diethylamino-2-pentyne
Inchi:	InChI=1S/C9H17N/c1-4-7-8-9-10(5-2)6-3/h4-6,9H2,1-3H3
InchiKey:	GLYRYDQBPLDITK-UHFFFAOYSA-N
Formula:	C9H17N
SMILES:	CCC#CCN(CC)CC
Mol. weight [g/mol]:	139.24

Physical Properties

Property code	Value	Unit	Source
af	0.2970		Cheméo Relay (1.0)
gf	338.48	kJ/mol	Joback Method
hf	121.89	kJ/mol	Cheméo Relay (1.0)
hfus	25.21	kJ/mol	Joback Method
hvap	50.01	kJ/mol	Cheméo Relay (1.0)
ie	7.67	eV	Cheméo Relay (1.0)
log10ws	-1.15		Cheméo Relay (1.0)
logp	1.742		Crippen Method
mcvol	139.050	ml/mol	McGowan Method
pc	2701.41	kPa	Joback Method
tb	423.66	K	Cheméo Relay (1.0)
tc	609.43	K	Cheméo Relay (1.0)
tf	192.37	K	Cheméo Relay (1.0)
vc	0.488	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	277.22	J/mol×K	426.76	Joback Method
cpg	291.60	J/mol×K	457.44	Joback Method
cpg	305.36	J/mol×K	488.11	Joback Method
cpg	318.51	J/mol×K	518.79	Joback Method
cpg	331.07	J/mol×K	549.46	Joback Method
cpg	343.07	J/mol×K	580.14	Joback Method
cpg	354.52	J/mol×K	610.81	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C73117109&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

af:	Acentric Factor
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
ie:	Ionization energy
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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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