3-Diethylamino-1-phenylpropyne

Other names: 2-Propynylamine, N,N-diethyl-3-phenyl-
N,N-Diethyl-3-phenyl-2-propynylamine
Inchi: InChI=1S/C13H17N/c1-3-14(4-2)12-8-11-13-9-6-5-7-10-13/h5-7,9-10H,3-4,12H2,1-2H3
InchiKey: NGTMXVYXKKHDPO-UHFFFAOYSA-N
Formula: C13H17N
SMILES: CCN(CC)CC#Cc1ccccc1
Mol. weight [g/mol]: 187.28
CAS: 22396-72-1

Physical Properties

Property code	Value	Unit	Source
gf	484.57	kJ/mol	Joback Method
hf	264.71	kJ/mol	Joback Method
hfus	29.61	kJ/mol	Joback Method
hvap	51.00	kJ/mol	Joback Method
log10ws	-2.83		Crippen Method
logp	2.380		Crippen Method
mcvol	171.650	ml/mol	McGowan Method
pc	2558.51	kPa	Joback Method
tb	544.96	K	Joback Method
tc	763.78	K	Joback Method
tf	401.26	K	Joback Method
vc	0.635	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	393.74	J/mol×K	544.96	Joback Method
cpg	411.34	J/mol×K	581.43	Joback Method
cpg	427.84	J/mol×K	617.90	Joback Method
cpg	443.30	J/mol×K	654.37	Joback Method
cpg	457.78	J/mol×K	690.84	Joback Method
cpg	471.32	J/mol×K	727.31	Joback Method
cpg	483.98	J/mol×K	763.78	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	418.50 ± 0.50	K	2.70	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C22396721&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

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