

4-(N-methylbenzylamino)-1-butyne

Inchi:	InChI=1S/C12H15N/c1-3-4-10-13(2)11-12-8-6-5-7-9-12/h1,5-9H,4,10-11H2,2H3
InchiKey:	BIJSXEQPHWTNCP-UHFFFAOYSA-N
Formula:	C12H15N
SMILES:	C#CCCN(C)Cc1ccccc1
Mol. weight [g/mol]:	173.25
CAS:	15240-91-2

Physical Properties

Property code	Value	Unit	Source
gf	496.42	kJ/mol	Joback Method
hf	304.95	kJ/mol	Joback Method
hfus	26.87	kJ/mol	Joback Method
hvap	46.48	kJ/mol	Joback Method
log10ws	-2.81		Crippen Method
logp	2.142		Crippen Method
mvol	157.560	ml/mol	McGowan Method
pc	2790.61	kPa	Joback Method
tb	503.20	K	Joback Method
tc	714.05	K	Joback Method
tf	330.86	K	Joback Method
vc	0.580	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	344.60	J/mol×K	503.20	Joback Method
cpg	361.03	J/mol×K	538.34	Joback Method
cpg	376.41	J/mol×K	573.48	Joback Method
cpg	390.80	J/mol×K	608.62	Joback Method
cpg	404.25	J/mol×K	643.76	Joback Method
cpg	416.81	J/mol×K	678.91	Joback Method
cpg	428.55	J/mol×K	714.05	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C15240912&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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

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