Benzylamine,2, n-dimethyl-n-2-propynyl-

Inchi: InChI=1S/C12H15N/c1-4-9-13(3)10-12-8-6-5-7-11(12)2/h1,5-8H,9-10H2,2-3H3
InchiKey: BIEGPBZDKLCGIM-UHFFFAOYSA-N
Formula: C12H15N
SMILES: C#CCN(C)Cc1ccccc1C
Mol. weight [g/mol]: 173.25
CAS: 709-53-5

Physical Properties

Property code	Value	Unit	Source
gf	486.79	kJ/mol	Joback Method
hf	293.48	kJ/mol	Joback Method
hfus	26.48	kJ/mol	Joback Method
hvap	47.15	kJ/mol	Joback Method
log10ws	-2.87		Crippen Method
logp	2.060		Crippen Method
mcvol	157.560	ml/mol	McGowan Method
pc	2746.90	kPa	Joback Method
tb	508.18	K	Joback Method
tc	720.23	K	Joback Method
tf	343.38	K	Joback Method
vc	0.580	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	345.11	J/mol×K	508.18	Joback Method
cpg	361.14	J/mol×K	543.52	Joback Method
cpg	376.18	J/mol×K	578.86	Joback Method
cpg	390.28	J/mol×K	614.20	Joback Method
cpg	403.50	J/mol×K	649.54	Joback Method
cpg	415.87	J/mol×K	684.89	Joback Method
cpg	427.46	J/mol×K	720.23	Joback Method

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=C709535&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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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