Benzylamine, o-bromo-n-methyl-n-2-propynyl-

Inchi: InChI=1S/C11H12BrN/c1-3-8-13(2)9-10-6-4-5-7-11(10)12/h1,4-7H,8-9H2,2H3
InchiKey: RAQPZRZYBLVXPM-UHFFFAOYSA-N
Formula: C11H12BrN
SMILES: C#CCN(C)Cc1ccccc1Br
Mol. weight [g/mol]: 238.12
CAS: 879-95-8

Physical Properties

Property code	Value	Unit	Source
gf	492.69	kJ/mol	Joback Method
hf	340.45	kJ/mol	Joback Method
hfus	29.18	kJ/mol	Joback Method
hvap	51.35	kJ/mol	Joback Method
log10ws	-3.55		Crippen Method
logp	2.514		Crippen Method
mcvol	160.970	ml/mol	McGowan Method
pc	3291.59	kPa	Joback Method
tb	551.46	K	Joback Method
tc	782.16	K	Joback Method
tf	391.91	K	Joback Method
vc	0.586	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	340.92	J/mol×K	551.46	Joback Method
cpg	354.91	J/mol×K	589.91	Joback Method
cpg	367.87	J/mol×K	628.36	Joback Method
cpg	379.88	J/mol×K	666.81	Joback Method
cpg	391.01	J/mol×K	705.26	Joback Method
cpg	401.32	J/mol×K	743.71	Joback Method
cpg	410.90	J/mol×K	782.16	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C879958&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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume