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

Inchi: InChI=1S/C17H25NO/c1-4-6-7-10-14-19-17-12-9-8-11-16(17)15-18(3)13-5-2/h2,8-9,11-1
InchiKey: WEDCRZDESSVZGX-UHFFFAOYSA-N
Formula: C17H25NO
SMILES: C#CCN(C)Cc1ccccc1OCCCCCC
Mol. weight [g/mol]: 259.39
CAS: 56862-38-5

Physical Properties

Property code	Value	Unit	Source
gf	423.89	kJ/mol	Joback Method
hf	58.06	kJ/mol	Joback Method
hfus	40.62	kJ/mol	Joback Method
hvap	60.69	kJ/mol	Joback Method
log10ws	-4.60		Crippen Method
logp	3.711		Crippen Method
mcvol	233.880	ml/mol	McGowan Method
pc	1728.90	kPa	Joback Method
tb	645.00	K	Joback Method
tc	840.46	K	Joback Method
tf	421.96	K	Joback Method
vc	0.877	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	622.69	J/mol×K	645.00	Joback Method
cpg	640.91	J/mol×K	677.58	Joback Method
cpg	658.12	J/mol×K	710.15	Joback Method
cpg	674.38	J/mol×K	742.73	Joback Method
cpg	689.71	J/mol×K	775.31	Joback Method
cpg	704.17	J/mol×K	807.89	Joback Method
cpg	717.78	J/mol×K	840.46	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C56862385&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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