3-Dibutylamino-1-propyne

Inchi: InChI=1S/C11H21N/c1-4-7-10-12(9-6-3)11-8-5-2/h3H,4-5,7-11H2,1-2H3
InchiKey: XTEBRELWTGWYDE-UHFFFAOYSA-N
Formula: C11H21N
SMILES: C#CCN(CCCC)CCCC
Mol. weight [g/mol]: 167.29
CAS: 6336-58-9

Physical Properties

Property code	Value	Unit	Source
gf	375.59	kJ/mol	Joback Method
hf	89.06	kJ/mol	Joback Method
hfus	30.24	kJ/mol	Joback Method
hvap	41.98	kJ/mol	Joback Method
log10ws	-2.79		Crippen Method
logp	2.522		Crippen Method
mcvol	167.230	ml/mol	McGowan Method
pc	2208.29	kPa	Joback Method
tb	453.64	K	Joback Method
tc	624.36	K	Joback Method
tf	293.17	K	Joback Method
vc	0.631	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	361.18	J/mol×K	453.64	Joback Method
cpg	376.97	J/mol×K	482.09	Joback Method
cpg	392.07	J/mol×K	510.55	Joback Method
cpg	406.49	J/mol×K	539.00	Joback Method
cpg	420.26	J/mol×K	567.45	Joback Method
cpg	433.42	J/mol×K	595.91	Joback Method
cpg	445.97	J/mol×K	624.36	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6336589&Units=SI

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