allyl-n-butyl-amine

Inchi: InChI=1S/C7H15N/c1-3-5-7-8-6-4-2/h4,8H,2-3,5-7H2,1H3
InchiKey: SNAUETXKUXDMFB-UHFFFAOYSA-N
Formula: C7H15N
SMILES: C=CCNCCCC
Mol. weight [g/mol]: 113.20

Physical Properties

Property code	Value	Unit	Source
gf	185.29	kJ/mol	Joback Method
hf	-8.91	kJ/mol	Joback Method
hfus	17.71	kJ/mol	Joback Method
hvap	36.94	kJ/mol	Joback Method
log10ws	-1.80		Crippen Method
logp	1.562		Crippen Method
mcvol	115.170	ml/mol	McGowan Method
pc	2969.80	kPa	Joback Method
rinpol	837.00		NIST Webbook
rinpol	837.00		NIST Webbook
tb	406.41	K	Joback Method
tc	579.08	K	Joback Method
tf	219.55	K	Joback Method
vc	0.444	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	222.92	J/mol×K	406.41	Joback Method
cpg	234.93	J/mol×K	435.19	Joback Method
cpg	246.46	J/mol×K	463.97	Joback Method
cpg	257.50	J/mol×K	492.75	Joback Method
cpg	268.08	J/mol×K	521.52	Joback Method
cpg	278.21	J/mol×K	550.30	Joback Method
cpg	287.90	J/mol×K	579.08	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R521687&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume