2-Butyl-pyrrolidine

Other names: pyrrolidine, 2-butyl-
Inchi: InChI=1S/C8H17N/c1-2-3-5-8-6-4-7-9-8/h8-9H,2-7H2,1H3
InchiKey: CKHOSERPJPIUIL-UHFFFAOYSA-N
Formula: C8H17N
SMILES: CCCCC1CCCN1
Mol. weight [g/mol]: 127.23
CAS: 3446-98-8

Physical Properties

Property code	Value	Unit	Source
gf	140.74	kJ/mol	Joback Method
hf	-110.16	kJ/mol	Joback Method
hfus	20.00	kJ/mol	Joback Method
hvap	40.42	kJ/mol	Joback Method
log10ws	-2.37		Crippen Method
logp	1.929		Crippen Method
mcvol	122.700	ml/mol	McGowan Method
pc	3152.62	kPa	Joback Method
rinpol	1025.00		NIST Webbook
tb	446.27	K	Joback Method
tc	647.04	K	Joback Method
tf	295.85	K	Joback Method
vc	0.462	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	258.53	J/mol×K	446.27	Joback Method
cpg	275.18	J/mol×K	479.73	Joback Method
cpg	291.05	J/mol×K	513.19	Joback Method
cpg	306.17	J/mol×K	546.65	Joback Method
cpg	320.54	J/mol×K	580.11	Joback Method
cpg	334.20	J/mol×K	613.58	Joback Method
cpg	347.16	J/mol×K	647.04	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=C3446988&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume