2-Isobutyl-pyrrolidine

Inchi: InChI=1S/C8H17N/c1-7(2)6-8-4-3-5-9-8/h7-9H,3-6H2,1-2H3
InchiKey: GNUABXXBKUNKNU-UHFFFAOYSA-N
Formula: C8H17N
SMILES: CC(C)CC1CCCN1
Mol. weight [g/mol]: 127.23

Physical Properties

Property code	Value	Unit	Source
gf	138.30	kJ/mol	Joback Method
hf	-115.44	kJ/mol	Joback Method
hfus	16.48	kJ/mol	Joback Method
hvap	40.03	kJ/mol	Joback Method
log10ws	-2.13		Crippen Method
logp	1.785		Crippen Method
mcvol	122.700	ml/mol	McGowan Method
pc	3181.14	kPa	Joback Method
rinpol	981.00		NIST Webbook
rinpol	981.00		NIST Webbook
tb	445.83	K	Joback Method
tc	651.36	K	Joback Method
tf	280.85	K	Joback Method
vc	0.456	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	258.58	J/mol×K	445.83	Joback Method
cpg	275.72	J/mol×K	480.09	Joback Method
cpg	292.03	J/mol×K	514.34	Joback Method
cpg	307.54	J/mol×K	548.60	Joback Method
cpg	322.27	J/mol×K	582.85	Joback Method
cpg	336.23	J/mol×K	617.11	Joback Method
cpg	349.46	J/mol×K	651.36	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=R405753&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume