Pyrroline, 2-isobutyl

Inchi: InChI=1S/C8H15N/c1-7(2)6-8-4-3-5-9-8/h7H,3-6H2,1-2H3
InchiKey: HHQRWQQRDCVPQH-UHFFFAOYSA-N
Formula: C8H15N
SMILES: CC(C)CC1=NCCC1
Mol. weight [g/mol]: 125.21

Physical Properties

Property code	Value	Unit	Source
gf	195.41	kJ/mol	Joback Method
hf	-15.63	kJ/mol	Joback Method
hfus	11.79	kJ/mol	Joback Method
hvap	40.74	kJ/mol	Joback Method
log10ws	-1.99		Crippen Method
logp	2.267		Crippen Method
mcvol	118.400	ml/mol	McGowan Method
pc	3291.59	kPa	Joback Method
ripol	975.00		NIST Webbook
ripol	975.00		NIST Webbook
tb	459.79	K	Joback Method
tc	673.48	K	Joback Method
tf	264.88	K	Joback Method
vc	0.455	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	258.69	J/mol×K	459.79	Joback Method
cpg	275.46	J/mol×K	495.41	Joback Method
cpg	291.37	J/mol×K	531.02	Joback Method
cpg	306.44	J/mol×K	566.64	Joback Method
cpg	320.69	J/mol×K	602.25	Joback Method
cpg	334.13	J/mol×K	637.87	Joback Method
cpg	346.79	J/mol×K	673.48	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=R604405&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume