

2-Isopropyl-piperidine

Inchi:	InChI=1S/C8H17N/c1-7(2)8-5-3-4-6-9-8/h7-9H,3-6H2,1-2H3
InchiKey:	UGZMDPJPZIDCOA-UHFFFAOYSA-N
Formula:	C8H17N
SMILES:	CC(C)C1CCCCN1
Mol. weight [g/mol]:	127.23

Physical Properties

Property code	Value	Unit	Source
gf	126.20	kJ/mol	Joback Method
hf	-121.60	kJ/mol	Joback Method
hfus	14.38	kJ/mol	Joback Method
hvap	40.20	kJ/mol	Joback Method
log10ws	-2.13		Crippen Method
logp	1.785		Crippen Method
mcvol	122.700	ml/mol	McGowan Method
pc	3272.78	kPa	Joback Method
rinsol	975.00		NIST Webbook
tb	450.10	K	Joback Method
tc	663.96	K	Joback Method
tf	277.33	K	Joback Method
vc	0.448	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	258.00	J/molxK	450.10	Joback Method
cpg	276.21	J/molxK	485.74	Joback Method
cpg	293.54	J/molxK	521.39	Joback Method
cpg	310.00	J/molxK	557.03	Joback Method
cpg	325.61	J/molxK	592.67	Joback Method
cpg	340.39	J/molxK	628.32	Joback Method
cpg	354.35	J/molxK	663.96	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=R405773&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I

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
hvac:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mccol:	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

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