2-Acetylpiperidine

Inchi: InChI=1S/C7H13NO/c1-6(9)7-4-2-3-5-8-7/h7-8H,2-5H2,1H3
InchiKey: SHTKZOSFNVMLJZ-UHFFFAOYSA-N
Formula: C7H13NO
SMILES: CC(=O)C1CCCCN1
Mol. weight [g/mol]: 127.18
CAS: 97073-22-8

Physical Properties

Property code	Value	Unit	Source
gf	-8.70	kJ/mol	Joback Method
hf	-208.26	kJ/mol	Joback Method
hfus	16.91	kJ/mol	Joback Method
hvap	45.11	kJ/mol	Joback Method
log10ws	-1.23		Crippen Method
logp	0.717		Crippen Method
mcvol	110.180	ml/mol	McGowan Method
pc	3920.94	kPa	Joback Method
ripol	1571.00		NIST Webbook
tb	481.53	K	Joback Method
tc	704.57	K	Joback Method
tf	330.99	K	Joback Method
vc	0.404	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	237.38	J/mol×K	481.53	Joback Method
cpg	253.02	J/mol×K	518.70	Joback Method
cpg	267.83	J/mol×K	555.88	Joback Method
cpg	281.84	J/mol×K	593.05	Joback Method
cpg	295.05	J/mol×K	630.23	Joback Method
cpg	307.48	J/mol×K	667.40	Joback Method
cpg	319.13	J/mol×K	704.57	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=C97073228&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