2-propionylpiperidine

Inchi: InChI=1S/C7H13NO/c1-2-7(9)6-4-3-5-8-6/h6,8H,2-5H2,1H3
InchiKey: VZOCHZFQIYOLNB-UHFFFAOYSA-N
Formula: C7H13NO
SMILES: CCC(=O)C1CCCN1
Mol. weight [g/mol]: 127.18

Physical Properties

Property code	Value	Unit	Source
gf	3.40	kJ/mol	Joback Method
hf	-202.10	kJ/mol	Joback Method
hfus	19.01	kJ/mol	Joback Method
hvap	44.94	kJ/mol	Joback Method
log10ws	-1.23		Crippen Method
logp	0.717		Crippen Method
mcvol	110.180	ml/mol	McGowan Method
pc	3801.00	kPa	Joback Method
ripol	1638.00		NIST Webbook
ripol	1638.00		NIST Webbook
tb	477.26	K	Joback Method
tc	691.82	K	Joback Method
tf	334.51	K	Joback Method
vc	0.411	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	237.92	J/mol×K	477.26	Joback Method
cpg	252.55	J/mol×K	513.02	Joback Method
cpg	266.42	J/mol×K	548.78	Joback Method
cpg	279.55	J/mol×K	584.54	Joback Method
cpg	291.96	J/mol×K	620.30	Joback Method
cpg	303.66	J/mol×K	656.06	Joback Method
cpg	314.68	J/mol×K	691.82	Joback Method

Sources

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=R312186&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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

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