Pyrrolidine-5-one, 2-[3-hydroxypropyl]-

Other names: Pyrrolidin-5-one, 2-[3-hydroxypropyl]-
Inchi: InChI=1S/C7H13NO2/c9-5-1-2-6-3-4-7(10)8-6/h6,9H,1-5H2,(H,8,10)
InchiKey: CJGLHMSXEHVWKR-UHFFFAOYSA-N
Formula: C7H13NO2
SMILES: OCCCC1CCC(O)=N1
Mol. weight [g/mol]: 143.18
CAS: 80243-73-8

Physical Properties

Property code	Value	Unit	Source
gf	-91.92	kJ/mol	Joback Method
hf	-314.51	kJ/mol	Joback Method
hfus	21.97	kJ/mol	Joback Method
hvap	71.95	kJ/mol	Joback Method
log10ws	-1.01		Crippen Method
logp	0.878		Crippen Method
mcvol	116.050	ml/mol	McGowan Method
pc	4420.84	kPa	Joback Method
ripol	2167.00		NIST Webbook
tb	617.04	K	Joback Method
tc	804.22	K	Joback Method
tf	386.01	K	Joback Method
vc	0.442	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	323.98	J/mol×K	617.04	Joback Method
cpg	334.97	J/mol×K	648.24	Joback Method
cpg	345.38	J/mol×K	679.43	Joback Method
cpg	355.23	J/mol×K	710.63	Joback Method
cpg	364.53	J/mol×K	741.82	Joback Method
cpg	373.29	J/mol×K	773.02	Joback Method
cpg	381.50	J/mol×K	804.22	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C80243738&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

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