2-Pyrrolidinone, 5-(cyclohexylmethyl)-

Inchi: InChI=1S/C11H19NO/c13-11-7-6-10(12-11)8-9-4-2-1-3-5-9/h9-10H,1-8H2,(H,12,13)
InchiKey: KLRBTOVJAIAXOI-UHFFFAOYSA-N
Formula: C11H19NO
SMILES: OC1=NC(CC2CCCCC2)CC1
Mol. weight [g/mol]: 181.27
CAS: 14293-08-4

Physical Properties

Property code	Value	Unit	Source
gf	103.03	kJ/mol	Joback Method
hf	-190.52	kJ/mol	Joback Method
hfus	20.07	kJ/mol	Joback Method
hvap	64.61	kJ/mol	Joback Method
log10ws	-3.07		Crippen Method
logp	3.076		Crippen Method
mcvol	155.680	ml/mol	McGowan Method
pc	3173.97	kPa	Joback Method
rinpol	1477.00		NIST Webbook
tb	635.93	K	Joback Method
tc	856.29	K	Joback Method
tf	377.65	K	Joback Method
vc	0.580	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	457.57	J/mol×K	635.93	Joback Method
cpg	476.58	J/mol×K	672.66	Joback Method
cpg	494.34	J/mol×K	709.38	Joback Method
cpg	510.87	J/mol×K	746.11	Joback Method
cpg	526.22	J/mol×K	782.84	Joback Method
cpg	540.40	J/mol×K	819.56	Joback Method
cpg	553.45	J/mol×K	856.29	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=C14293084&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume