(5S,6R)-5,6-O-Isopropylidene-azepane-2-one

Inchi: InChI=1S/C9H15NO3/c1-9(2)12-6-3-4-8(11)10-5-7(6)13-9/h6-7H,3-5H2,1-2H3,(H,10,11)/
InchiKey: UDINENAKQQNEQK-RQJHMYQMSA-N
Formula: C9H15NO3
SMILES: CC1(C)OC2CCC(=O)NCC2O1
Mol. weight [g/mol]: 185.22

Physical Properties

Property code	Value	Unit	Source
gf	-122.32	kJ/mol	Joback Method
hf	-477.12	kJ/mol	Joback Method
hfus	26.77	kJ/mol	Joback Method
hvap	54.71	kJ/mol	Joback Method
log10ws	-1.35		Crippen Method
logp	0.417		Crippen Method
mcvol	139.240	ml/mol	McGowan Method
pc	3594.25	kPa	Joback Method
rinpol	1614.00		NIST Webbook
tb	601.72	K	Joback Method
tc	853.77	K	Joback Method
tf	459.04	K	Joback Method
vc	0.504	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	387.68	J/mol×K	601.72	Joback Method
cpg	406.57	J/mol×K	643.73	Joback Method
cpg	424.32	J/mol×K	685.74	Joback Method
cpg	441.06	J/mol×K	727.74	Joback Method
cpg	456.92	J/mol×K	769.75	Joback Method
cpg	472.01	J/mol×K	811.76	Joback Method
cpg	486.47	J/mol×K	853.77	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=R500333&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume