Azacyclotridecan-2-one

Other names:	1-Aza-2-cyclotridecanone
	2-Oxo-dodecamethylenimine
	2-azacyclotridecanone
	Aza-cyclotridecan-2-on
	Cyclododecalactam
	Dodecalactam
	Dodecanoic acid, 12-amino-, lactam
	Dodecanolactam
	Dodecyllactam
	Laurin lactam
	Laurinolactam
	Laurolactam
	Lauryl lactam
	NSC 77100
	cyclododecanone isooxime
	dodecane-12-lactam
	«omega»-Dodecalactam
	«omega»-Dodecanolactam
	«omega»-Laurolactam
Inchi:	InChI=1S/C12H23NO/c14-12-10-8-6-4-2-1-3-5-7-9-11-13-12/h1-11H2,(H,13,14)
InchiKey:	JHWNWJKBPDFINM-UHFFFAOYSA-N
Formula:	C12H23NO
SMILES:	O=C1CCCCCCCCCCCN1
Mol. weight [g/mol]:	197.32
CAS:	947-04-6

Physical Properties

Property code	Value	Unit	Source
gf	-37.26	kJ/mol	Joback Method
hf	-359.36	kJ/mol	Joback Method
hfus	12.00	kJ/mol	Joback Method
hvap	55.25	kJ/mol	Joback Method
log10ws	-3.70		Crippen Method
logp	3.017		Crippen Method
mcvol	180.630	ml/mol	McGowan Method
pc	2778.85	kPa	Joback Method
tb	644.44	K	Joback Method

tc	911.28	K	Joback Method
tf	385.23	K	Joback Method
tt	425.95	K	Solid-Liquid Equilibrium of Azacyclotridecan-2-one in 15 Pure Solvents from T = 273.15 to 323.15 K: Experimental Determination and Thermodynamic Modeling
vc	0.629	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	504.20	J/mol×K	644.44	Joback Method
cpg	531.53	J/mol×K	688.91	Joback Method
cpg	556.79	J/mol×K	733.39	Joback Method
cpg	579.90	J/mol×K	777.86	Joback Method
cpg	600.76	J/mol×K	822.34	Joback Method
cpg	619.26	J/mol×K	866.81	Joback Method
cpg	635.32	J/mol×K	911.28	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=C947046&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Solid-Liquid Equilibrium of Azacyclotridecan-2-one in 15 Pure Solvents from T = 273.15 to 323.15 K: Experimental Determination and Thermodynamic Modeling:	https://www.doi.org/10.1021/acs.jced.8b01193

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume