Cyclononanone

Inchi: InChI=1S/C9H16O/c10-9-7-5-3-1-2-4-6-8-9/h1-8H2
InchiKey: BAUZLFKYYIVGPM-UHFFFAOYSA-N
Formula: C9H16O
SMILES: O=C1CCCCCCCC1
Mol. weight [g/mol]: 140.22
CAS: 3350-30-9

Physical Properties

Property code	Value	Unit	Source
affp	852.60	kJ/mol	NIST Webbook
basg	822.80	kJ/mol	NIST Webbook
chs	-5493.40 ± 1.50	kJ/mol	NIST Webbook
gf	-101.83	kJ/mol	Joback Method
hf	-279.70 ± 1.70	kJ/mol	NIST Webbook
hfs	-334.90 ± 1.60	kJ/mol	NIST Webbook
hfus	1.60	kJ/mol	NIST Webbook
hvap	53.10 ± 0.60	kJ/mol	NIST Webbook
log10ws	-2.76		Crippen Method
logp	2.690		Crippen Method
mcvol	128.380	ml/mol	McGowan Method
pc	3325.84	kPa	Joback Method
rinpol	1239.00		NIST Webbook
rinpol	1239.00		NIST Webbook
rinpol	1256.00		NIST Webbook
rinpol	1252.00		NIST Webbook
tb	493.60 ± 1.50	K	NIST Webbook
tc	753.74	K	Joback Method
tf	305.10 ± 2.00	K	NIST Webbook
vc	0.457	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	312.55	J/mol×K	550.76	Joback Method

cpg	332.55	J/mol×K	591.36	Joback Method
cpg	351.43	J/mol×K	631.95	Joback Method
cpg	369.15	J/mol×K	672.55	Joback Method
cpg	385.69	J/mol×K	713.14	Joback Method
cpg	291.46	J/mol×K	510.17	Joback Method
cpg	401.02	J/mol×K	753.74	Joback Method
hfust	14.70	kJ/mol	247.00	NIST Webbook
hfust	1.60	kJ/mol	298.00	NIST Webbook
hvapt	51.40	kJ/mol	373.00	NIST Webbook
sfust	59.50	J/mol×K	247.00	NIST Webbook
sfust	5.40	J/mol×K	298.00	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	369.20	K	2.40	NIST Webbook
tbrp	367.20	K	1.60	NIST Webbook

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=C3350309&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

affp: Proton affinity
basg: Gas basicity
chs: Standard solid enthalpy of combustion
cpg: Ideal gas heat capacity
gf: Standard Gibbs free energy of formation
hf: Enthalpy of formation at standard conditions
hfs: Solid phase enthalpy of formation at standard conditions

hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
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
sfust:	Entropy of fusion at a given temperature
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume