2(1H)-AZOCINONE, HEXAHYDRO-

Other names:	Hexahydro-2(1H)-azocinone 2-Ketoheptamethyleneimine «omega»-Heptanolactam 2(1H)-Azocinone, hexahydro- 7-Aminoheptanoic acid lactam Azacyclooctan-2-one Enantholactam «omega»-Enantholactam «zeta»-Enantholactam 7-Heptanelactam Octahydroazocin-2-one Oenantholactam 2-Perhydroazocinone Suberonisoxim 2H-Azocin-2-one, hexahydro- NSC 77088 hexahydroazocin-2(1H)-one
Inchi:	InChI=1S/C7H13NO/c9-7-5-3-1-2-4-6-8-7/h1-6H2,(H,8,9)
InchiKey:	CJYXCQLOZNIMFP-UHFFFAOYSA-N
Formula:	C7H13NO
SMILES:	O=C1CCCCCCN1
Mol. weight [g/mol]:	127.19

Physical Properties

Property code	Value	Unit	Source
af	0.3965		Cheméo Relay (1.0)
chs	-4263.90 ± 1.30	kJ/mol	NIST Webbook
gf	-18.86	kJ/mol	Joback Method
hf	-293.92	kJ/mol	Cheméo Relay (1.0)
hfus	9.55	kJ/mol	Joback Method
hvap	65.76	kJ/mol	Cheméo Relay (1.0)
ie	9.19	eV	NIST Webbook
log10ws	-0.16		Cheméo Relay (1.0)
logp	1.067		Crippen Method
mcvol	110.180	ml/mol	McGowan Method
pc	4205.63	kPa	Joback Method
tb	540.29	K	Cheméo Relay (1.0)

tc	773.95	K	Cheméo Relay (1.0)
tf	308.20 ± 0.50	K	NIST Webbook
tt	310.29 ± 0.02	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	244.25	J/mol×K	508.69	Joback Method
cpg	262.25	J/mol×K	550.15	Joback Method
cpg	279.38	J/mol×K	591.61	Joback Method
cpg	295.60	J/mol×K	633.08	Joback Method
cpg	310.86	J/mol×K	674.54	Joback Method
cpg	325.13	J/mol×K	716.00	Joback Method
cpg	338.35	J/mol×K	757.46	Joback Method
hfust	13.78	kJ/mol	310.30	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	422.20	K	1.30	NIST Webbook

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C673665&Units=SI

Legend

af:	Acentric Factor
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
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature