

2-Oxonanone

Other names:	«eta»-Caprylolactone Octanoic acid, 8-hydroxy-, «eta»-lactone
Inchi:	InChI=1S/C8H14O2/c9-8-6-4-2-1-3-5-7-10-8/h1-7H2
InchiKey:	ZYDGQQTXLBN SGJ-UHFFFAOYSA-N
Formula:	C8H14O2
SMILES:	O=C1CCCCCCCCO1
Mol. weight [g/mol]:	142.20
CAS:	5698-29-3

Physical Properties

Property code	Value	Unit	Source
gf	-196.37	kJ/mol	Joback Method
hf	-434.00 ± 3.00	kJ/mol	NIST Webbook
hfl	-487.00 ± 3.00	kJ/mol	NIST Webbook
hfus	8.43	kJ/mol	Joback Method
hvap	53.00 ± 1.00	kJ/mol	NIST Webbook
hvap	53.00	kJ/mol	NIST Webbook
hvap	52.80 ± 1.30	kJ/mol	NIST Webbook
log10ws	-1.93		Crippen Method
logp	1.884		Crippen Method
mvol	120.160	ml/mol	McGowan Method
pc	3686.49	kPa	Joback Method
tb	514.24	K	Joback Method
tc	759.92	K	Joback Method
tf	275.77	K	Joback Method
vc	0.421	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	276.72	J/mol×K	514.24	Joback Method
cpg	296.14	J/mol×K	555.19	Joback Method
cpg	314.55	J/mol×K	596.13	Joback Method
cpg	331.92	J/mol×K	637.08	Joback Method

cpg	348.21	J/mol×K	678.02	Joback Method
cpg	363.38	J/mol×K	718.97	Joback Method
cpg	377.40	J/mol×K	759.92	Joback Method
hvapt	48.90 ± 0.20	kJ/mol	362.50	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=C5698293&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
hfl:	Liquid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

Latest version available from:

<https://www.chemeo.com/cid/58-806-3/2-Oxonanone.pdf>

Generated by Cheméo on 2024-04-19 22:13:20.932482076 +0000 UTC m=+15854049.853059391.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.