

1,4-CYCLOOCTANEDIONE

Inchi:	InChI=1S/C8H12O2/c9-7-3-1-2-4-8(10)6-5-7/h1-6H2
InchiKey:	LZTHLBQVLFQNKK-UHFFFAOYSA-N
Formula:	C8H12O2
SMILES:	O=C1CCCCC(=O)CC1
Mol. weight [g/mol]:	140.18

Physical Properties

Property code	Value	Unit	Source
af	0.4308		Cheméo Relay (1.0)
gf	-220.74	kJ/mol	Joback Method
hf	-385.34	kJ/mol	Cheméo Relay (1.0)
hfus	2.06	kJ/mol	Joback Method
hvap	61.35	kJ/mol	Cheméo Relay (1.0)
ie	9.17	eV	Cheméo Relay (1.0)
log10ws	-0.59		Cheméo Relay (1.0)
logp	1.479		Crippen Method
mcvol	115.860	ml/mol	McGowan Method
pc	3773.04	kPa	Joback Method
tb	507.69	K	Cheméo Relay (1.0)
tc	728.79	K	Cheméo Relay (1.0)
tf	363.94	K	Cheméo Relay (1.0)
vc	0.384	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	275.89	J/mol×K	550.84	Joback Method
cpg	294.34	J/mol×K	593.44	Joback Method
cpg	311.86	J/mol×K	636.03	Joback Method
cpg	328.36	J/mol×K	678.63	Joback Method
cpg	343.76	J/mol×K	721.23	Joback Method
cpg	358.00	J/mol×K	763.82	Joback Method
cpg	371.00	J/mol×K	806.42	Joback Method
hfust	11.92	kJ/mol	341.20	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C55794451&Units=SI
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):	

Legend

af:	Acentric Factor
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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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