

(Z)-1,5-Octadien-3-one

Other names:	(Z)-Octa-1,5-dien-3-one 1,5(Z)-octadien-3-one octa-1,cis-5-dien-3-one
Inchi:	InChI=1S/C8H12O/c1-3-5-6-7-8(9)4-2/h4-6H,2-3,7H2,1H3/b6-5-
InchiKey:	VWYBQOFZVSND AW-WAYWQWQ TSA-N
Formula:	C8H12O
SMILES:	C=CC(=O)CC=CCC
Mol. weight [g/mol]:	124.18

Physical Properties

Property code	Value	Unit	Source
gf	55.62	kJ/mol	Joback Method
hf	-78.38	kJ/mol	Joback Method
hfus	17.00	kJ/mol	Joback Method
hvap	39.44	kJ/mol	Joback Method
log10ws	-2.16		Crippen Method
logp	2.098		Crippen Method
mcvol	116.550	ml/mol	McGowan Method
pc	2989.32	kPa	Joback Method
rinpol	984.00		NIST Webbook
rinpol	984.00		NIST Webbook
rinpol	984.00		NIST Webbook
rinpol	976.00		NIST Webbook
rinpol	984.00		NIST Webbook
rinpol	985.00		NIST Webbook
rinpol	982.00		NIST Webbook
rinpol	984.00		NIST Webbook
rinpol	980.00		NIST Webbook
rinpol	984.00		NIST Webbook
rinpol	983.00		NIST Webbook
rinpol	985.00		NIST Webbook
rinpol	983.00		NIST Webbook
rinpol	963.00		NIST Webbook
rinpol	979.00		NIST Webbook
rinpol	983.00		NIST Webbook
rinpol	986.00		NIST Webbook
rinpol	980.00		NIST Webbook

rinpol	992.00	NIST Webbook
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rinpol	982.00	NIST Webbook
rinpol	978.00	NIST Webbook
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ripol	1408.00		NIST Webbook
ripol	1395.00		NIST Webbook
ripol	1373.00		NIST Webbook
ripol	1406.00		NIST Webbook
ripol	1379.00		NIST Webbook
ripol	1375.00		NIST Webbook
ripol	1367.00		NIST Webbook
tb	437.15	K	Joback Method
tc	625.01	K	Joback Method
tf	223.01	K	Joback Method
vc	0.451	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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cpg	223.71	J/molxK	437.15	Joback Method
cpg	235.28	J/molxK	468.46	Joback Method
cpg	246.25	J/molxK	499.77	Joback Method
cpg	256.66	J/molxK	531.08	Joback Method
cpg	266.53	J/molxK	562.39	Joback Method
cpg	275.88	J/molxK	593.70	Joback Method
cpg	284.73	J/molxK	625.01	Joback Method
dvisc	0.0035628	Paxs	223.01	Joback Method
dvisc	0.0016740	Paxs	258.70	Joback Method
dvisc	0.0009446	Paxs	294.39	Joback Method
dvisc	0.0006033	Paxs	330.08	Joback Method
dvisc	0.0004205	Paxs	365.77	Joback Method
dvisc	0.0003125	Paxs	401.46	Joback Method
dvisc	0.0002438	Paxs	437.15	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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=C65767228&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature

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

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