3,5-Octadien-2-one

Other names:	3,5-Octadiene-2-one
	Octa-3,5-dien-2-one
	3,5-Octadienone
Inchi:	InChI=1S/C8H12O/c1-3-4-5-6-7-8(2)9/h4-7H,3H2,1-2H3
InchiKey:	LWRKMRFJEUFXIB-UHFFFAOYSA-N
Formula:	C8H12O
SMILES:	CCC=CC=CC(C)=O
Mol. weight [g/mol]:	124.18
CAS:	38284-27-4

Physical Properties

Property code	Value	Unit	Source
gf	48.00	kJ/mol	Joback Method
hf	-86.59	kJ/mol	Joback Method
hfus	18.48	kJ/mol	Joback Method
hvap	40.06	kJ/mol	Joback Method
log10ws	-2.16		Crippen Method
logp	2.098		Crippen Method
mcvol	116.550	ml/mol	McGowan Method
pc	3022.28	kPa	Joback Method
rinpol	1096.00		NIST Webbook
rinpol	1070.00		NIST Webbook
rinpol	1107.00		NIST Webbook
rinpol	1098.00		NIST Webbook
rinpol	1107.00		NIST Webbook
rinpol	1090.00		NIST Webbook
rinpol	1069.00		NIST Webbook
rinpol	1098.00		NIST Webbook
rinpol	1070.00		NIST Webbook
rinpol	1072.00		NIST Webbook
rinpol	1048.00		NIST Webbook
rinpol	1063.00		NIST Webbook
rinpol	1065.00		NIST Webbook
rinpol	1040.00		NIST Webbook
rinpol	1040.00		NIST Webbook
rinpol	1056.00		NIST Webbook
rinpol	1072.00		NIST Webbook

rinpol	1043.00	NIST Webbook
rinpol	1098.00	NIST Webbook
rinpol	1074.00	NIST Webbook
rinpol	1067.00	NIST Webbook
rinpol	1052.00	NIST Webbook
rinpol	1063.00	NIST Webbook
rinpol	1068.00	NIST Webbook
rinpol	1048.00	NIST Webbook
rinpol	1049.00	NIST Webbook
rinpol	1070.00	NIST Webbook
rinpol	1071.00	NIST Webbook
rinpol	1048.00	NIST Webbook
rinpol	1072.00	NIST Webbook
rinpol	1072.00	NIST Webbook
rinpol	1102.00	NIST Webbook
rinpol	1093.00	NIST Webbook
rinpol	1099.00	NIST Webbook
rinpol	1081.00	NIST Webbook
rinpol	1067.00	NIST Webbook
rinpol	1098.00	NIST Webbook
rinpol	1081.00	NIST Webbook
rinpol	1092.00	NIST Webbook
rinpol	1076.00	NIST Webbook
rinpol	1099.00	NIST Webbook
rinpol	1074.00	NIST Webbook
ripol	1536.00	NIST Webbook
ripol	1531.00	NIST Webbook
ripol	1569.00	NIST Webbook
ripol	1521.00	NIST Webbook
ripol	1522.00	NIST Webbook
ripol	1522.00	NIST Webbook
ripol	1520.00	NIST Webbook
ripol	1524.00	NIST Webbook
ripol	1531.00	NIST Webbook
ripol	1569.00	NIST Webbook
ripol	1531.00	NIST Webbook
ripol	1505.00	NIST Webbook
ripol	1516.00	NIST Webbook
ripol	1536.00	NIST Webbook
ripol	1518.00	NIST Webbook
ripol	1521.00	NIST Webbook
ripol	1516.00	NIST Webbook
ripol	1516.00	NIST Webbook
ripol	1521.00	NIST Webbook

ripol	1567.00		NIST Webbook
ripol	1536.00		NIST Webbook
tb	444.63	K	Joback Method
tc	637.71	K	Joback Method
tf	219.69	K	Joback Method
vc	0.450	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	223.73	J/mol×K	444.63	Joback Method
cpg	235.56	J/mol×K	476.81	Joback Method
cpg	246.73	J/mol×K	508.99	Joback Method
cpg	257.29	J/mol×K	541.17	Joback Method
cpg	267.25	J/mol×K	573.35	Joback Method
cpg	276.65	J/mol×K	605.53	Joback Method
cpg	285.54	J/mol×K	637.71	Joback Method
dvisc	0.0037387	Pa×s	219.69	Joback Method
dvisc	0.0016178	Pa×s	257.18	Joback Method
dvisc	0.0008664	Pa×s	294.67	Joback Method
dvisc	0.0005342	Pa×s	332.16	Joback Method
dvisc	0.0003633	Pa×s	369.65	Joback Method
dvisc	0.0002653	Pa×s	407.14	Joback Method
dvisc	0.0002043	Pa×s	444.63	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C38284274&Units=SI

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

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

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