(E,Z)-3,5-Octadien-2-one

Other names:	(E)-3,(Z)-5-octadien-2-one
	trans, cis-3,5-octadien-2-one
	3,5-octadien-2-one (E, Z)
	(E,Z)-Octa-3,5-dien-2-one
	trans-3,cis-5-octadien-2-one
Inchi:	InChI=1S/C8H12O/c1-3-4-5-6-7-8(2)9/h4-7H,3H2,1-2H3/b5-4-,7-6+
InchiKey:	LWRKMRFJEUFXIB-SCFJQAPRSA-N
Formula:	C8H12O
SMILES:	CCC=CC=CC(C)=O
Mol. weight [g/mol]:	124.18

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	1095.00		NIST Webbook
rinpol	1050.00		NIST Webbook
rinpol	1096.00		NIST Webbook
rinpol	1083.00		NIST Webbook
rinpol	1098.00		NIST Webbook
rinpol	1098.00		NIST Webbook
rinpol	1095.00		NIST Webbook
rinpol	1095.00		NIST Webbook
rinpol	1076.00		NIST Webbook
rinpol	1070.20		NIST Webbook
rinpol	1095.00		NIST Webbook
rinpol	1053.00		NIST Webbook
rinpol	1104.00		NIST Webbook
rinpol	1098.00		NIST Webbook
rinpol	1068.00		NIST Webbook
rinpol	1096.00		NIST Webbook

rinpol	1096.00		NIST Webbook
rinpol	1092.00		NIST Webbook
ripol	1493.00		NIST Webbook
ripol	1493.00		NIST Webbook
ripol	1513.00		NIST Webbook
ripol	1517.00		NIST Webbook
ripol	1529.00		NIST Webbook
ripol	1539.00		NIST Webbook
ripol	1545.00		NIST Webbook
ripol	1552.00		NIST Webbook
ripol	1556.00		NIST Webbook
ripol	1484.00		NIST Webbook
ripol	1482.00		NIST Webbook
ripol	1482.00		NIST Webbook
ripol	1500.00		NIST Webbook
ripol	1504.00		NIST Webbook
ripol	1515.00		NIST Webbook
ripol	1520.00		NIST Webbook
ripol	1480.00		NIST Webbook
ripol	1509.00		NIST Webbook
ripol	1516.00		NIST Webbook
ripol	1525.00		NIST Webbook
ripol	1488.00		NIST Webbook
ripol	1529.00		NIST Webbook
ripol	1488.00		NIST Webbook
ripol	1517.00		NIST Webbook
ripol	1513.00		NIST Webbook
ripol	1484.00		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

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R149270&Units=SI

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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