3-Octen-2-one, (E)-

Other names:	trans-3-Octen-2-one
	E-3-Octen-2-one
	(E)-Oct-3-en-2-one
	3(E),3-Octen-2-one
Inchi:	InChI=1S/C8H14O/c1-3-4-5-6-7-8(2)9/h6-7H,3-5H2,1-2H3/b7-6+
InchiKey:	ZCFOBLITZWHNNC-VOTSOKGWSA-N
Formula:	C8H14O
SMILES:	CCCCC=CC(C)=O
Mol. weight [g/mol]:	126.20
CAS:	18402-82-9

Physical Properties

Property code	Value	Unit	Source
gf	-32.22	kJ/mol	Joback Method
hf	-203.81	kJ/mol	Joback Method
hfus	18.28	kJ/mol	Joback Method
hvap	40.11	kJ/mol	Joback Method
log10ws	-2.30		Crippen Method
logp	2.322		Crippen Method
mcvol	120.850	ml/mol	McGowan Method
pc	2856.62	kPa	Joback Method
rinpol	1031.00		NIST Webbook
rinpol	1034.00		NIST Webbook
rinpol	1040.00		NIST Webbook
rinpol	1036.00		NIST Webbook
rinpol	1032.00		NIST Webbook
ripol	1411.00		NIST Webbook
ripol	1396.00		NIST Webbook
ripol	1392.00		NIST Webbook
tb	440.47	K	Joback Method
tc	624.44	K	Joback Method
tf	224.77	K	Joback Method
vc	0.469	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	239.73	J/mol×K	440.47	Joback Method
cpg	251.92	J/mol×K	471.13	Joback Method
cpg	263.55	J/mol×K	501.79	Joback Method
cpg	274.62	J/mol×K	532.46	Joback Method
cpg	285.17	J/mol×K	563.12	Joback Method
cpg	295.21	J/mol×K	593.78	Joback Method
cpg	304.76	J/mol×K	624.44	Joback Method
dvisc	0.0040418	Pa×s	224.77	Joback Method
dvisc	0.0018362	Pa×s	260.72	Joback Method
dvisc	0.0010100	Pa×s	296.67	Joback Method
dvisc	0.0006321	Pa×s	332.62	Joback Method
dvisc	0.0004335	Pa×s	368.57	Joback Method
dvisc	0.0003179	Pa×s	404.52	Joback Method
dvisc	0.0002453	Pa×s	440.47	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C18402829&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