(Z)-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-SREVYHEPSA-N
Formula: C8H14O
SMILES: CCCCC=CC(C)=O
Mol. weight [g/mol]: 126.20

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	1055.00		NIST Webbook
rinpol	1023.00		NIST Webbook
rinpol	1023.00		NIST Webbook
ripol	1285.00		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=R235648&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