(E)-1,5-octadien-3-one

Inchi: InChI=1S/C8H12O/c1-3-5-6-7-8(9)4-2/h4-6H,2-3,7H2,1H3/b6-5+
InchiKey: VWYBQOFZVSNDAW-AATRIKPKSA-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	988.00		NIST Webbook
tb	437.15	K	Joback Method
tc	625.01	K	Joback Method
tf	223.01	K	Joback Method
vc	0.451	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	223.71	J/mol×K	437.15	Joback Method
cpg	235.28	J/mol×K	468.46	Joback Method
cpg	246.25	J/mol×K	499.77	Joback Method
cpg	256.66	J/mol×K	531.08	Joback Method
cpg	266.53	J/mol×K	562.39	Joback Method
cpg	275.88	J/mol×K	593.70	Joback Method
cpg	284.73	J/mol×K	625.01	Joback Method
dvisc	0.0035628	Pa×s	223.01	Joback Method
dvisc	0.0016740	Pa×s	258.70	Joback Method

dvisc	0.0009446	Pa×s	294.39	Joback Method
dvisc	0.0006033	Pa×s	330.08	Joback Method
dvisc	0.0004205	Pa×s	365.77	Joback Method
dvisc	0.0003125	Pa×s	401.46	Joback Method
dvisc	0.0002438	Pa×s	437.15	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R339121&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

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