7-Octen-2-one

Inchi: InChI=1S/C8H14O/c1-3-4-5-6-7-8(2)9/h3H,1,4-7H2,2H3
InchiKey: RXHCEQYNSQNEOK-UHFFFAOYSA-N
Formula: C8H14O
SMILES: C=CCCCCC(C)=O
Mol. weight [g/mol]: 126.20
CAS: 3664-60-6

Physical Properties

Property code	Value	Unit	Source
gf	-24.60	kJ/mol	Joback Method
hf	-195.60	kJ/mol	Joback Method
hfus	16.79	kJ/mol	Joback Method
hvap	39.48	kJ/mol	Joback Method
log10ws	-2.30		Crippen Method
logp	2.322		Crippen Method
mcvol	120.850	ml/mol	McGowan Method
pc	2826.33	kPa	Joback Method
rinpol	1097.00		NIST Webbook
tb	432.99	K	Joback Method
tc	611.99	K	Joback Method
tf	228.09	K	Joback Method
vc	0.470	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	239.51	J/mol×K	432.99	Joback Method
cpg	251.42	J/mol×K	462.82	Joback Method
cpg	262.81	J/mol×K	492.66	Joback Method
cpg	273.71	J/mol×K	522.49	Joback Method
cpg	284.13	J/mol×K	552.32	Joback Method
cpg	294.08	J/mol×K	582.16	Joback Method
cpg	303.57	J/mol×K	611.99	Joback Method
dvisc	0.0038763	Pa×s	228.09	Joback Method

dvisc	0.0019045	Pa×s	262.24	Joback Method
dvisc	0.0011022	Pa×s	296.39	Joback Method
dvisc	0.0007142	Pa×s	330.54	Joback Method
dvisc	0.0005020	Pa×s	364.69	Joback Method
dvisc	0.0003748	Pa×s	398.84	Joback Method
dvisc	0.0002930	Pa×s	432.99	Joback Method

Sources

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=C3664606&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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