8-HYDROXY-2-OCTANONE

Inchi: InChI=1S/C8H16O2/c1-8(10)6-4-2-3-5-7-9/h9H,2-7H2,1H3
InchiKey: UMDPPTMXBUCHCM-UHFFFAOYSA-N
Formula: C8H16O2
SMILES: CC(=O)CCCCCCO
Mol. weight [g/mol]: 144.21

Physical Properties

Property code	Value	Unit	Source
af	0.7414		Cheméo Relay (1.0)
gf	-249.26	kJ/mol	Joback Method
hf	-490.69	kJ/mol	Cheméo Relay (1.0)
hfus	22.16	kJ/mol	Joback Method
hvap	77.70	kJ/mol	Cheméo Relay (1.0)
ie	9.37	eV	Cheméo Relay (1.0)
log10ws	-0.70		Cheméo Relay (1.0)
logp	1.518		Crippen Method
mcvol	131.020	ml/mol	McGowan Method
pc	2982.79	kPa	Joback Method
ripol	2181.00		NIST Webbook
tb	522.17	K	Cheméo Relay (1.0)
tc	707.74	K	Cheméo Relay (1.0)
tf	297.62	K	Cheméo Relay (1.0)
vc	0.483	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	309.45	J/mol×K	528.49	Joback Method
cpg	320.30	J/mol×K	556.64	Joback Method
cpg	330.71	J/mol×K	584.79	Joback Method
cpg	340.68	J/mol×K	612.94	Joback Method
cpg	350.23	J/mol×K	641.09	Joback Method
cpg	359.37	J/mol×K	669.24	Joback Method
cpg	368.11	J/mol×K	697.39	Joback Method

dvisc	0.0161114	Pa×s	290.67	Joback Method
dvisc	0.0046128	Pa×s	330.31	Joback Method
dvisc	0.0017266	Pa×s	369.94	Joback Method
dvisc	0.0007817	Pa×s	409.58	Joback Method
dvisc	0.0004070	Pa×s	449.22	Joback Method
dvisc	0.0002356	Pa×s	488.85	Joback Method
dvisc	0.0001480	Pa×s	528.49	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C25368541&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

af:	Acentric Factor
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
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume