

5-Hydroxy-4-octanone

Other names:	Butyroin 4-Octanone, 5-hydroxy- 5-Octanol-4-one 5-hydroxyoctan-4-one
Inchi:	InChI=1S/C8H16O2/c1-3-5-7(9)8(10)6-4-2/h7,9H,3-6H2,1-2H3
InchiKey:	BVEYJWQCMVMAR-UHFFFAOYSA-N
Formula:	C8H16O2
SMILES:	CCCC(=O)C(O)CCC
Mol. weight [g/mol]:	144.21
CAS:	496-77-5

Physical Properties

Property code	Value	Unit	Source
gf	-251.70	kJ/mol	Joback Method
hf	-478.54	kJ/mol	Joback Method
hfus	18.64	kJ/mol	Joback Method
hvap	56.44	kJ/mol	Joback Method
log10ws	-1.83		Crippen Method
logp	1.517		Crippen Method
mcvol	131.020	ml/mol	McGowan Method
pc	3009.03	kPa	Joback Method
tb	458.20	K	NIST Webbook
tc	700.14	K	Joback Method
tf	275.67	K	Joback Method
vc	0.502	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	309.75	J/mol×K	528.05	Joback Method
cpg	320.87	J/mol×K	556.73	Joback Method
cpg	331.52	J/mol×K	585.41	Joback Method
cpg	341.71	J/mol×K	614.10	Joback Method
cpg	351.46	J/mol×K	642.78	Joback Method

cpg	360.77	J/mol×K	671.46	Joback Method
cpg	369.66	J/mol×K	700.14	Joback Method
dvisc	0.0284980	Pa×s	275.67	Joback Method
dvisc	0.0065326	Pa×s	317.73	Joback Method
dvisc	0.0021132	Pa×s	359.80	Joback Method
dvisc	0.0008658	Pa×s	401.86	Joback Method
dvisc	0.0004201	Pa×s	443.92	Joback Method
dvisc	0.0002310	Pa×s	485.99	Joback Method
dvisc	0.0001397	Pa×s	528.05	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	356.00 ± 3.00	K	1.60	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C496775&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

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

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