BUTYROIN

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:	BVEYJWQCMOVMAR-UHFFFAOYSA-N
Formula:	C8H16O2
SMILES:	CCCC(=O)C(O)CCC
Mol. weight [g/mol]:	144.21

Physical Properties

Property code	Value	Unit	Source
hf	-501.34	kJ/mol	Cheméo Relay (1.0)
hfus	18.64	kJ/mol	Joback Method
hvap	63.17	kJ/mol	Cheméo Relay (1.0)
ie	9.40	eV	Cheméo Relay (1.0)
log10ws	-0.80		Cheméo Relay (1.0)
logp	1.517		Crippen Method
mcvol	131.020	ml/mol	McGowan Method
tb	458.20	K	NIST Webbook
tc	655.13	K	Cheméo Relay (1.0)
tf	304.27	K	Cheméo Relay (1.0)
vc	0.484	m3/kmol	Cheméo Relay (1.0)

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

Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C496775&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
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):

Legend

cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
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
tb: Normal Boiling Point Temperature

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