2-pentanon-3-ol

Other names: 3-hydroxypentan-2-one
2-pentanon-3-ol
2-Pentanone, 3-hydroxy-
Inchi: InChI=1S/C5H10O2/c1-3-5(7)4(2)6/h5,7H,3H2,1-2H3
InchiKey: HDKKRASBPHFULQ-UHFFFAOYSA-N
Formula: C5H10O2
SMILES: CCC(O)C(C)=O
Mol. weight [g/mol]: 102.13

Physical Properties

Property code	Value	Unit	Source
hf	-442.80	kJ/mol	Cheméo Relay (1.0)
hfus	10.87	kJ/mol	Joback Method
hvap	56.23	kJ/mol	Cheméo Relay (1.0)
ie	9.65	eV	Cheméo Relay (1.0)
log10ws	0.70		Cheméo Relay (1.0)
logp	0.346		Crippen Method
mcvol	88.750	ml/mol	McGowan Method
rinpol	768.00		NIST Webbook
rinpol	783.00		NIST Webbook
rinpol	838.00		NIST Webbook
rinpol	815.00		NIST Webbook
ripol	1366.00		NIST Webbook
ripol	1368.00		NIST Webbook
ripol	1327.00		NIST Webbook
ripol	1346.00		NIST Webbook
ripol	1340.00		NIST Webbook
ripol	1330.00		NIST Webbook
ripol	1338.00		NIST Webbook
ripol	1345.00		NIST Webbook
ripol	1338.00		NIST Webbook
ripol	1349.00		NIST Webbook
ripol	1355.00		NIST Webbook
ripol	1344.00		NIST Webbook
ripol	1338.00		NIST Webbook
tb	421.46	K	Cheméo Relay (1.0)
tc	608.54	K	Cheméo Relay (1.0)

tf	283.39	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	183.94	J/mol×K	459.41	Joback Method
cpg	191.99	J/mol×K	488.80	Joback Method
cpg	199.72	J/mol×K	518.19	Joback Method
cpg	207.12	J/mol×K	547.58	Joback Method
cpg	214.20	J/mol×K	576.97	Joback Method
cpg	220.97	J/mol×K	606.37	Joback Method
cpg	227.44	J/mol×K	635.76	Joback Method
dvisc	0.0540168	Pa×s	241.86	Joback Method
dvisc	0.0120393	Pa×s	278.12	Joback Method
dvisc	0.0037936	Pa×s	314.38	Joback Method
dvisc	0.0015179	Pa×s	350.63	Joback Method
dvisc	0.0007211	Pa×s	386.89	Joback Method
dvisc	0.0003892	Pa×s	423.15	Joback Method
dvisc	0.0002315	Pa×s	459.41	Joback Method

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C3142663&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

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
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point