3-hydroxyoctan-2-one

Other names: 2-octanon-3-ol
Inchi: InChI=1S/C8H16O2/c1-3-4-5-6-8(10)7(2)9/h8,10H,3-6H2,1-2H3
InchiKey: QWEHQNZGVUHHME-UHFFFAOYSA-N
Formula: C8H16O2
SMILES: CCCCCC(O)C(C)=O
Mol. weight [g/mol]: 144.21

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
rinpol	1073.00		NIST Webbook
rinpol	1105.00		NIST Webbook
rinpol	1105.00		NIST Webbook
ripol	1655.00		NIST Webbook
tb	528.05	K	Joback Method
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	360.77	J/mol×K	671.46	Joback Method
cpg	351.46	J/mol×K	642.78	Joback Method
cpg	341.71	J/mol×K	614.10	Joback Method
cpg	331.52	J/mol×K	585.41	Joback Method

cpg	320.87	J/mol×K	556.73	Joback Method
cpg	369.66	J/mol×K	700.14	Joback Method
dvisc	0.0001397	Pa×s	528.05	Joback Method
dvisc	0.0002310	Pa×s	485.99	Joback Method
dvisc	0.0004201	Pa×s	443.92	Joback Method
dvisc	0.0008658	Pa×s	401.86	Joback Method
dvisc	0.0021132	Pa×s	359.80	Joback Method
dvisc	0.0065326	Pa×s	317.73	Joback Method
dvisc	0.0284980	Pa×s	275.67	Joback Method

Sources

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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R210441&Units=SI

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
ripol: Polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume

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