

3-hexanon-2-ol

Other names:	2-Hydroxyhexan-3-one
Inchi:	InChI=1S/C6H12O2/c1-3-4-6(8)5(2)7/h5,7H,3-4H2,1-2H3
InchiKey:	ZWBUSAWJHMPOEJ-UHFFFAOYSA-N
Formula:	C6H12O2
SMILES:	CCCC(=O)C(C)O
Mol. weight [g/mol]:	116.16
CAS:	54073-43-7

Physical Properties

Property code	Value	Unit	Source
gf	-268.54	kJ/mol	Joback Method
hf	-437.26	kJ/mol	Joback Method
hfus	13.46	kJ/mol	Joback Method
hvap	51.99	kJ/mol	Joback Method
log10ws	-0.99		Crippen Method
logp	0.736		Crippen Method
mcvol	102.840	ml/mol	McGowan Method
pc	3759.17	kPa	Joback Method
rinpol	895.50		NIST Webbook
rinpol	895.50		NIST Webbook
tb	482.29	K	Joback Method
tc	657.19	K	Joback Method
tf	253.13	K	Joback Method
vc	0.391	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	223.83	J/mol×K	482.29	Joback Method
cpg	266.02	J/mol×K	628.04	Joback Method
cpg	258.31	J/mol×K	598.89	Joback Method
cpg	250.24	J/mol×K	569.74	Joback Method
cpg	241.81	J/mol×K	540.59	Joback Method
cpg	233.01	J/mol×K	511.44	Joback Method

cpg	273.38	J/mol×K	657.19	Joback Method
dvisc	0.0001967	Pa×s	482.29	Joback Method
dvisc	0.0003288	Pa×s	444.10	Joback Method
dvisc	0.0006050	Pa×s	405.90	Joback Method
dvisc	0.0012640	Pa×s	367.71	Joback Method
dvisc	0.0031323	Pa×s	329.52	Joback Method
dvisc	0.0098475	Pa×s	291.32	Joback Method
dvisc	0.0437428	Pa×s	253.13	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C54073437&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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