3-heptanon-2-ol

Inchi: InChI=1S/C7H14O2/c1-3-4-5-7(9)6(2)8/h6,8H,3-5H2,1-2H3
InchiKey: KTKQJWVLAMSBTM-UHFFFAOYSA-N
Formula: C7H14O2
SMILES: CCCCC(=O)C(C)O
Mol. weight [g/mol]: 130.18

Physical Properties

Property code	Value	Unit	Source
gf	-260.12	kJ/mol	Joback Method
hf	-457.90	kJ/mol	Joback Method
hfus	16.05	kJ/mol	Joback Method
hvap	54.21	kJ/mol	Joback Method
log10ws	-1.41		Crippen Method
logp	1.127		Crippen Method
mcvol	116.930	ml/mol	McGowan Method
pc	3352.86	kPa	Joback Method
ripol	1551.00		NIST Webbook
ripol	1551.00		NIST Webbook
tb	505.17	K	Joback Method
tc	678.63	K	Joback Method
tf	264.40	K	Joback Method
vc	0.447	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	265.80	J/mol×K	505.17	Joback Method
cpg	312.64	J/mol×K	649.72	Joback Method
cpg	304.09	J/mol×K	620.81	Joback Method
cpg	295.14	J/mol×K	591.90	Joback Method
cpg	285.78	J/mol×K	562.99	Joback Method
cpg	276.01	J/mol×K	534.08	Joback Method
cpg	320.81	J/mol×K	678.63	Joback Method
dvisc	0.0001662	Pa×s	505.17	Joback Method

dvisc	0.0002761	Pa×s	465.04	Joback Method
dvisc	0.0005050	Pa×s	424.91	Joback Method
dvisc	0.0010476	Pa×s	384.78	Joback Method
dvisc	0.0025758	Pa×s	344.66	Joback Method
dvisc	0.0080276	Pa×s	304.53	Joback Method
dvisc	0.0353274	Pa×s	264.40	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R241059&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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