

3-(hydroxymethyl)nonan-2-one

Inchi:	InChI=1S/C10H20O2/c1-3-4-5-6-7-10(8-11)9(2)12/h10-11H,3-8H2,1-2H3
InchiKey:	DIZUHEORFPDTIQ-UHFFFAOYSA-N
Formula:	C10H20O2
SMILES:	CCCCCCC(CO)C(C)=O
Mol. weight [g/mol]:	172.26
CAS:	67801-33-6

Physical Properties

Property code	Value	Unit	Source
gf	-234.86	kJ/mol	Joback Method
hf	-519.82	kJ/mol	Joback Method
hfus	23.82	kJ/mol	Joback Method
hvap	60.89	kJ/mol	Joback Method
log10ws	-2.31		Crippen Method
logp	2.154		Crippen Method
mcvol	159.200	ml/mol	McGowan Method
pc	2462.92	kPa	Joback Method
rinpol	1093.00		NIST Webbook
rinpol	1093.00		NIST Webbook
tb	573.81	K	Joback Method
tc	743.57	K	Joback Method
tf	298.21	K	Joback Method
vc	0.615	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	403.15	J/mol×K	573.81	Joback Method
cpg	415.84	J/mol×K	602.10	Joback Method
cpg	427.99	J/mol×K	630.40	Joback Method
cpg	439.61	J/mol×K	658.69	Joback Method
cpg	450.71	J/mol×K	686.99	Joback Method
cpg	461.31	J/mol×K	715.28	Joback Method
cpg	471.43	J/mol×K	743.57	Joback Method

dvisc	0.0185428	Paxs	298.21	Joback Method
dvisc	0.0043186	Paxs	344.14	Joback Method
dvisc	0.0014176	Paxs	390.08	Joback Method
dvisc	0.0005884	Paxs	436.01	Joback Method
dvisc	0.0002888	Paxs	481.94	Joback Method
dvisc	0.0001605	Paxs	527.88	Joback Method
dvisc	0.0000979	Paxs	573.81	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C67801336&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

Legend

cp_g:	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
h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀ws:	Log ₁₀ of Water solubility in mol/l
log_p:	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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