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]: 172.27

Physical Properties

Property code	Value	Unit	Source
af	0.7199		Cheméo Relay (1.0)
gf	-234.86	kJ/mol	Joback Method
hf	-521.90	kJ/mol	Cheméo Relay (1.0)
hfus	23.82	kJ/mol	Joback Method
hvap	74.66	kJ/mol	Cheméo Relay (1.0)
ie	9.34	eV	Cheméo Relay (1.0)
log10ws	-1.68		Cheméo Relay (1.0)
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	530.47	K	Cheméo Relay (1.0)
tc	713.40	K	Cheméo Relay (1.0)
tf	265.12	K	Cheméo Relay (1.0)
vc	0.567	m3/kmol	Cheméo Relay (1.0)

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	Pa×s	298.21	Joback Method
dvisc	0.0043186	Pa×s	344.14	Joback Method
dvisc	0.0014176	Pa×s	390.08	Joback Method
dvisc	0.0005884	Pa×s	436.01	Joback Method
dvisc	0.0002888	Pa×s	481.94	Joback Method
dvisc	0.0001605	Pa×s	527.88	Joback Method
dvisc	0.0000979	Pa×s	573.81	Joback Method

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C67801336&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

af: Acentric Factor
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
ie: Ionization energy
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