

3-octanon-2-ol

Inchi:	InChI=1S/C8H16O2/c1-3-4-5-6-8(10)7(2)9/h7,9H,3-6H2,1-2H3
InchiKey:	BNHJODMDMOKFFL-UHFFFAOYSA-N
Formula:	C8H16O2
SMILES:	CCCCC(=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
ripol	1647.00		NIST Webbook
ripol	1647.00		NIST Webbook
tb	528.05	K	Joback Method
tc	700.14	K	Joback Method
tf	275.67	K	Joback Method
vc	0.502	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	309.75	J/mol×K	528.05	Joback Method
cpg	320.87	J/mol×K	556.73	Joback Method
cpg	331.52	J/mol×K	585.41	Joback Method
cpg	341.71	J/mol×K	614.10	Joback Method
cpg	351.46	J/mol×K	642.78	Joback Method
cpg	360.77	J/mol×K	671.46	Joback Method
cpg	369.66	J/mol×K	700.14	Joback Method
dvisc	0.0284980	Paxs	275.67	Joback Method

dvisc	0.0065326	Paxs	317.73	Joback Method
dvisc	0.0021132	Paxs	359.80	Joback Method
dvisc	0.0008658	Paxs	401.86	Joback Method
dvisc	0.0004201	Paxs	443.92	Joback Method
dvisc	0.0002310	Paxs	485.99	Joback Method
dvisc	0.0001397	Paxs	528.05	Joback Method

Sources

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=R241168&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
hvap:	Enthalpy of vaporization at standard conditions
log₁₀ws:	Log ₁₀ 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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