

3-nonanon-2-ol

Inchi:	InChI=1S/C9H18O2/c1-3-4-5-6-7-9(11)8(2)10/h8,10H,3-7H2,1-2H3
InchiKey:	GHAYRYHCWULLDR-UHFFFAOYSA-N
Formula:	C9H18O2
SMILES:	CCCCCCC(=O)C(C)O
Mol. weight [g/mol]:	158.24

Physical Properties

Property code	Value	Unit	Source
gf	-243.28	kJ/mol	Joback Method
hf	-499.18	kJ/mol	Joback Method
hfus	21.23	kJ/mol	Joback Method
hvap	58.66	kJ/mol	Joback Method
log10ws	-2.25		Crippen Method
logp	1.907		Crippen Method
mcvol	145.110	ml/mol	McGowan Method
pc	2715.50	kPa	Joback Method
ripol	1757.00		NIST Webbook
ripol	1757.00		NIST Webbook
tb	550.93	K	Joback Method
tc	721.77	K	Joback Method
tf	286.94	K	Joback Method
vc	0.558	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	355.57	J/molxK	550.93	Joback Method
cpg	410.35	J/molxK	693.29	Joback Method
cpg	400.35	J/molxK	664.82	Joback Method
cpg	389.89	J/molxK	636.35	Joback Method
cpg	378.95	J/molxK	607.88	Joback Method
cpg	367.51	J/molxK	579.40	Joback Method
cpg	419.88	J/molxK	721.77	Joback Method
dvisc	0.0001171	Paxs	550.93	Joback Method

dvisc	0.0001927	Paxs	506.93	Joback Method
dvisc	0.0003486	Paxs	462.93	Joback Method
dvisc	0.0007142	Paxs	418.94	Joback Method
dvisc	0.0017314	Paxs	374.94	Joback Method
dvisc	0.0053119	Paxs	330.94	Joback Method
dvisc	0.0229838	Paxs	286.94	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R241153&Units=SI

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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