

(±)-octan-3-ol

Other names:	3-Octanol
Inchi:	InChI=1S/C8H18O/c1-3-5-6-7-8(9)4-2/h8-9H,3-7H2,1-2H3
InchiKey:	NMRPBPVERJPACX-UHFFFAOYSA-N
Formula:	C8H18O
SMILES:	CCCCC(O)CC
Mol. weight [g/mol]:	130.23
CAS:	20296-29-1

Physical Properties

Property code	Value	Unit	Source
gf	-122.78	kJ/mol	Joback Method
hf	-365.96	kJ/mol	Joback Method
hfus	17.04	kJ/mol	Joback Method
hvap	67.90 ± 0.30	kJ/mol	NIST Webbook
log10ws	-2.55		Crippen Method
logp	2.338		Crippen Method
mcvol	129.450	ml/mol	McGowan Method
pc	2811.36	kPa	Joback Method
tb	448.20	K	NIST Webbook
tc	637.10	K	Joback Method
tf	225.74	K	Joback Method
vc	0.496	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	324.43	J/mol×K	555.64	Joback Method
cpg	354.79	J/mol×K	637.10	Joback Method
cpg	345.08	J/mol×K	609.94	Joback Method
cpg	334.96	J/mol×K	582.79	Joback Method
cpg	290.23	J/mol×K	474.18	Joback Method
cpg	302.08	J/mol×K	501.33	Joback Method
cpg	313.47	J/mol×K	528.49	Joback Method
dvisc	0.0001689	Pa×s	474.18	Joback Method

dvisc	0.0013956	Pa×s	349.96	Joback Method
dvisc	0.0005948	Pa×s	391.37	Joback Method
dvisc	0.0002984	Pa×s	432.77	Joback Method
dvisc	0.1178389	Pa×s	225.74	Joback Method
dvisc	0.0169844	Pa×s	267.15	Joback Method
dvisc	0.0041171	Pa×s	308.55	Joback Method
hvapt	58.80	kJ/mol	399.00	NIST Webbook
hvapt	54.50	kJ/mol	408.00	NIST Webbook
hvapt	64.10	kJ/mol	381.50	NIST Webbook
hvapt	71.60	kJ/mol	300.50	NIST Webbook

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=C20296291&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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