

# Octane

**Other names:** Oktan; Oktanen; Ottani; UN 1262; n-C8H18; n-Octane.

**InChI:** InChI=1S/C8H18/c1-3-5-7-8-6-4-2/h3-8H2,1-2H3

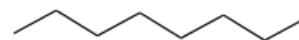
**InChI Key:** TVMXDCGIABBOFY-UHFFFAOYSA-N

**Formula:** C8H18

**SMILES:** CCCCCCCC

**Molecular Weight:** 114.23

**CAS:** 111-65-9



## Physical Properties

Property	Value	Unit	Source
$\Delta_c H^\circ_{\text{liquid}}$	$-5470.30 \pm 1.60$	kJ/mol	NIST Webbook
$\Delta_c H^\circ_{\text{liquid}}$	$-5470.71 \pm 0.67$	kJ/mol	NIST Webbook
$\Delta_c H^\circ_{\text{liquid}}$	-5466.60	kJ/mol	NIST Webbook
$\Delta_c H^\circ_{\text{liquid}}$	$-5471.80 \pm 5.40$	kJ/mol	NIST Webbook
$\Delta_c H^\circ_{\text{liquid}}$	-5441.30	kJ/mol	NIST Webbook
$\Delta_c H^\circ_{\text{liquid}}$	-5270.40	kJ/mol	NIST Webbook
$\Delta_f G^\circ$	16.48	kJ/mol	Joback Method
$\Delta_f H^\circ_{\text{gas}}$	-208.70	kJ/mol	NIST Webbook
$\Delta_f H^\circ_{\text{gas}}$	$-208.40 \pm 0.67$	kJ/mol	NIST Webbook
$\Delta_f H^\circ_{\text{liquid}}$	$-250.30 \pm 1.80$	kJ/mol	NIST Webbook
$\Delta_f H^\circ_{\text{liquid}}$	$-250.00 \pm 0.84$	kJ/mol	NIST Webbook
$\Delta_{\text{fus}} H^\circ$	16.48	kJ/mol	Joback Method
$\Delta_{\text{vap}} H^\circ$	41.53	kJ/mol	NIST Webbook
$\Delta_{\text{vap}} H^\circ$	41.60	kJ/mol	NIST Webbook
$\Delta_{\text{vap}} H^\circ$	$41.50 \pm 0.10$	kJ/mol	NIST Webbook
$\Delta_{\text{vap}} H^\circ$	$41.50 \pm 0.10$	kJ/mol	NIST Webbook
$\Delta_{\text{vap}} H^\circ$	41.50	kJ/mol	NIST Webbook

Property	Value	Unit	Source
$\Delta_{\text{vap}} H^\circ$	41.60 ± 0.08	kJ/mol	NIST Webbook
$\Delta_{\text{vap}} H^\circ$	41.60 ± 0.08	kJ/mol	NIST Webbook
$\Delta_{\text{vap}} H^\circ$	41.50 ± 0.10	kJ/mol	NIST Webbook
$\Delta_{\text{vap}} H^\circ$	41.48	kJ/mol	NIST Webbook
$\Delta_{\text{vap}} H^\circ$	34.00	kJ/mol	NIST Webbook
IE	9.80 ± 0.15	eV	NIST Webbook
IE	10.01	eV	NIST Webbook
IE	9.80 ± 0.10	eV	NIST Webbook
IE	9.71 ± 0.15	eV	NIST Webbook
IE	9.79	eV	NIST Webbook
IE	10.25	eV	NIST Webbook
$\log P_{\text{oct/wat}}$	3.367		Crippen Method
$P_c$	2490.00 ± 30.00	kPa	NIST Webbook
$P_c$	2495.00 ± 20.00	kPa	NIST Webbook
$P_c$	2487.00	kPa	NIST Webbook
$P_c$	2480.00 ± 5.00	kPa	NIST Webbook
$P_c$	2490.00 ± 30.00	kPa	NIST Webbook
$P_c$	2486.93 ± 17.23	kPa	NIST Webbook
$P_c$	2486.20 ± 40.53	kPa	NIST Webbook
$P_c$	2488.00 ± 40.53	kPa	NIST Webbook
$P_c$	2492.59 ± 50.66	kPa	NIST Webbook
$P_c$	2497.10 ± 20.00	kPa	NIST Webbook
$P_c$	2497.12 ± 19.99	kPa	NIST Webbook
$P_c$	2470.00 ± 98.07	kPa	NIST Webbook
$S^\circ_{\text{gas}}$	467.06 ± 0.92	J/mol×K	NIST Webbook
$S^\circ_{\text{liquid}}$	361.20	J/mol×K	NIST Webbook
$S^\circ_{\text{liquid}}$	359.80	J/mol×K	NIST Webbook
$S^\circ_{\text{liquid}}$	359.80	J/mol×K	NIST Webbook

Property	Value	Unit	Source
$T_{\text{boil}}$	$398.80 \pm 0.20$	K	NIST Webbook
$T_{\text{boil}}$	$398.80 \pm 0.20$	K	NIST Webbook
$T_{\text{boil}}$	398.90	K	NIST Webbook
$T_{\text{boil}}$	$398.73 \pm 0.10$	K	NIST Webbook
$T_{\text{boil}}$	398.80	K	NIST Webbook
$T_{\text{boil}}$	$398.76 \pm 0.20$	K	NIST Webbook
$T_{\text{boil}}$	$398.96 \pm 0.20$	K	NIST Webbook
$T_{\text{boil}}$	$398.96 \pm 0.50$	K	NIST Webbook
$T_{\text{boil}}$	$398.93 \pm 0.08$	K	NIST Webbook
$T_{\text{boil}}$	$398.70 \pm 0.50$	K	NIST Webbook
$T_{\text{boil}}$	$398.75 \pm 0.15$	K	NIST Webbook
$T_{\text{boil}}$	$398.55 \pm 0.20$	K	NIST Webbook
$T_{\text{boil}}$	$398.12 \pm 0.20$	K	NIST Webbook
$T_{\text{boil}}$	$398.77 \pm 0.10$	K	NIST Webbook
$T_{\text{boil}}$	$398.95 \pm 0.40$	K	NIST Webbook
$T_{\text{boil}}$	$398.76 \pm 0.20$	K	NIST Webbook
$T_{\text{boil}}$	$398.75 \pm 0.50$	K	NIST Webbook
$T_{\text{boil}}$	$398.55 \pm 0.30$	K	NIST Webbook
$T_{\text{boil}}$	$398.77 \pm 0.15$	K	NIST Webbook
$T_{\text{boil}}$	$398.27 \pm 0.30$	K	NIST Webbook
$T_{\text{boil}}$	$399.00 \pm 0.60$	K	NIST Webbook
$T_{\text{boil}}$	$398.40 \pm 1.00$	K	NIST Webbook
$T_{\text{boil}}$	$398.85 \pm 0.25$	K	NIST Webbook
$T_{\text{boil}}$	$398.82 \pm 0.30$	K	NIST Webbook
$T_{\text{boil}}$	$399.15 \pm 1.50$	K	NIST Webbook
$T_{\text{boil}}$	$397.80 \pm 0.30$	K	NIST Webbook
$T_{\text{boil}}$	$396.40 \pm 2.00$	K	NIST Webbook
$T_{\text{boil}}$	$398.85 \pm 0.40$	K	NIST Webbook

Property	Value	Unit	Source
$T_{\text{boil}}$	$399.09 \pm 0.30$	K	NIST Webbook
$T_{\text{boil}}$	$398.75 \pm 0.10$	K	NIST Webbook
$T_{\text{boil}}$	$398.81 \pm 0.44$	K	NIST Webbook
$T_{\text{boil}}$	$398.55 \pm 0.30$	K	NIST Webbook
$T_{\text{boil}}$	$398.71 \pm 0.20$	K	NIST Webbook
$T_{\text{boil}}$	$398.80 \pm 0.40$	K	NIST Webbook
$T_{\text{boil}}$	$398.95 \pm 0.50$	K	NIST Webbook
$T_{\text{boil}}$	$393.15 \pm 3.00$	K	NIST Webbook
$T_{\text{boil}}$	$398.81 \pm 0.10$	K	NIST Webbook
$T_{\text{boil}}$	$398.90 \pm 0.20$	K	NIST Webbook
$T_{\text{boil}}$	$398.25 \pm 0.30$	K	NIST Webbook
$T_{\text{boil}}$	$398.62 \pm 0.30$	K	NIST Webbook
$T_{\text{boil}}$	$397.85 \pm 0.30$	K	NIST Webbook
$T_{\text{boil}}$	$397.20 \pm 2.00$	K	NIST Webbook
$T_{\text{boil}}$	$398.75 \pm 0.30$	K	NIST Webbook
$T_{\text{boil}}$	$398.80 \pm 0.40$	K	NIST Webbook
$T_{\text{boil}}$	$398.85 \pm 0.50$	K	NIST Webbook
$T_{\text{boil}}$	$397.35 \pm 0.50$	K	NIST Webbook
$T_{\text{boil}}$	$398.75 \pm 0.30$	K	NIST Webbook
$T_{\text{boil}}$	$398.90 \pm 0.30$	K	NIST Webbook
$T_{\text{boil}}$	$398.75 \pm 0.40$	K	NIST Webbook
$T_{\text{boil}}$	$398.81 \pm 0.01$	K	NIST Webbook
$T_{\text{boil}}$	$397.65 \pm 0.50$	K	NIST Webbook
$T_{\text{boil}}$	$397.40 \pm 1.00$	K	NIST Webbook
$T_{\text{boil}}$	$398.15 \pm 2.00$	K	NIST Webbook
$T_{\text{boil}}$	$398.70 \pm 0.20$	K	NIST Webbook
$T_{\text{boil}}$	$398.95 \pm 0.50$	K	NIST Webbook
$T_{\text{boil}}$	$398.90 \pm 0.20$	K	NIST Webbook

Property	Value	Unit	Source
$T_{\text{boil}}$	$398.75 \pm 0.30$	K	NIST Webbook
$T_{\text{boil}}$	$398.81 \pm 0.10$	K	NIST Webbook
$T_{\text{boil}}$	$398.80 \pm 0.30$	K	NIST Webbook
$T_{\text{boil}}$	$397.15 \pm 1.00$	K	NIST Webbook
$T_{\text{boil}}$	$398.75 \pm 0.20$	K	NIST Webbook
$T_{\text{boil}}$	$401.65 \pm 0.50$	K	NIST Webbook
$T_{\text{boil}}$	$398.75 \pm 0.30$	K	NIST Webbook
$T_{\text{boil}}$	$398.90 \pm 0.20$	K	NIST Webbook
$T_{\text{boil}}$	$398.81 \pm 0.20$	K	NIST Webbook
$T_{\text{boil}}$	$398.95 \pm 0.20$	K	NIST Webbook
$T_{\text{boil}}$	$398.80 \pm 0.05$	K	NIST Webbook
$T_{\text{boil}}$	$398.55 \pm 0.50$	K	NIST Webbook
$T_{\text{boil}}$	$398.15 \pm 0.60$	K	NIST Webbook
$T_{\text{boil}}$	$396.00 \pm 2.00$	K	NIST Webbook
$T_{\text{boil}}$	$398.55 \pm 0.50$	K	NIST Webbook
$T_{\text{boil}}$	$398.75 \pm 0.50$	K	NIST Webbook
$T_{\text{boil}}$	$398.74 \pm 0.10$	K	NIST Webbook
$T_{\text{boil}}$	$398.35 \pm 0.30$	K	NIST Webbook
$T_{\text{boil}}$	$398.55 \pm 0.50$	K	NIST Webbook
$T_{\text{boil}}$	$398.74 \pm 0.15$	K	NIST Webbook
$T_{\text{boil}}$	$397.75 \pm 0.50$	K	NIST Webbook
$T_{\text{boil}}$	$398.95 \pm 0.20$	K	NIST Webbook
$T_{\text{boil}}$	$398.15 \pm 1.00$	K	NIST Webbook
$T_{\text{boil}}$	$397.65 \pm 0.30$	K	NIST Webbook
$T_{\text{boil}}$	$399.00 \pm 0.70$	K	NIST Webbook
$T_{\text{boil}}$	$399.00 \pm 1.00$	K	NIST Webbook
$T_{\text{boil}}$	$398.15 \pm 1.00$	K	NIST Webbook
$T_{\text{boil}}$	$398.95 \pm 0.30$	K	NIST Webbook

Property	Value	Unit	Source
$T_{\text{boil}}$	$398.15 \pm 2.00$	K	NIST Webbook
$T_{\text{boil}}$	$398.95 \pm 0.30$	K	NIST Webbook
$T_{\text{boil}}$	$398.64 \pm 0.10$	K	NIST Webbook
$T_{\text{boil}}$	$398.45 \pm 0.50$	K	NIST Webbook
$T_{\text{boil}}$	$396.70 \pm 1.50$	K	NIST Webbook
$T_{\text{c}}$	$568.70 \pm 0.30$	K	NIST Webbook
$T_{\text{c}}$	$568.50 \pm 1.00$	K	NIST Webbook
$T_{\text{c}}$	$568.60 \pm 0.30$	K	NIST Webbook
$T_{\text{c}}$	$568.65 \pm 0.20$	K	NIST Webbook
$T_{\text{c}}$	$568.80 \pm 0.60$	K	NIST Webbook
$T_{\text{c}}$	568.70	K	NIST Webbook
$T_{\text{c}}$	$568.92 \pm 0.10$	K	NIST Webbook
$T_{\text{c}}$	$568.60 \pm 0.20$	K	NIST Webbook
$T_{\text{c}}$	568.80	K	NIST Webbook
$T_{\text{c}}$	$568.80 \pm 0.70$	K	NIST Webbook
$T_{\text{c}}$	$568.80 \pm 0.20$	K	NIST Webbook
$T_{\text{c}}$	$568.80 \pm 0.40$	K	NIST Webbook
$T_{\text{c}}$	$569.00 \pm 0.30$	K	NIST Webbook
$T_{\text{c}}$	$569.00 \pm 0.40$	K	NIST Webbook
$T_{\text{c}}$	$568.80 \pm 0.20$	K	NIST Webbook
$T_{\text{c}}$	$568.75 \pm 0.30$	K	NIST Webbook
$T_{\text{c}}$	$568.74 \pm 0.40$	K	NIST Webbook
$T_{\text{c}}$	$568.77 \pm 0.40$	K	NIST Webbook
$T_{\text{c}}$	$568.56 \pm 0.20$	K	NIST Webbook
$T_{\text{c}}$	$569.15 \pm 0.60$	K	NIST Webbook
$T_{\text{c}}$	$569.40 \pm 1.00$	K	NIST Webbook
$T_{\text{c}}$	$569.35 \pm 0.50$	K	NIST Webbook
$T_{\text{c}}$	$569.60 \pm 1.00$	K	NIST Webbook

Property	Value	Unit	Source
$T_{\text{fus}}$	$216.32 \pm 0.10$	K	NIST Webbook
$T_{\text{fus}}$	$216.36 \pm 0.20$	K	NIST Webbook
$T_{\text{fus}}$	$216.35 \pm 0.15$	K	NIST Webbook
$T_{\text{fus}}$	$216.34 \pm 0.02$	K	NIST Webbook
$T_{\text{fus}}$	$216.35 \pm 0.15$	K	NIST Webbook
$T_{\text{fus}}$	$216.35 \pm 0.10$	K	NIST Webbook
$T_{\text{fus}}$	$216.34 \pm 0.15$	K	NIST Webbook
$T_{\text{fus}}$	$216.35 \pm 0.10$	K	NIST Webbook
$T_{\text{fus}}$	$216.35 \pm 0.15$	K	NIST Webbook
$T_{\text{fus}}$	$216.35 \pm 0.10$	K	NIST Webbook
$T_{\text{fus}}$	$216.36 \pm 0.19$	K	NIST Webbook
$T_{\text{fus}}$	$216.28 \pm 0.03$	K	NIST Webbook
$T_{\text{fus}}$	$216.34 \pm 0.15$	K	NIST Webbook
$T_{\text{fus}}$	$216.34 \pm 0.10$	K	NIST Webbook
$T_{\text{fus}}$	$216.30 \pm 0.20$	K	NIST Webbook
$T_{\text{fus}}$	$216.35 \pm 0.20$	K	NIST Webbook
$T_{\text{fus}}$	$216.26 \pm 0.08$	K	NIST Webbook
$T_{\text{fus}}$	$216.15 \pm 0.30$	K	NIST Webbook
$T_{\text{fus}}$	$216.59 \pm 0.20$	K	NIST Webbook
$T_{\text{fus}}$	$215.85 \pm 0.30$	K	NIST Webbook
$T_{\text{fus}}$	$216.59 \pm 0.20$	K	NIST Webbook
$T_{\text{fus}}$	$216.34 \pm 0.01$	K	NIST Webbook
$T_{\text{fus}}$	$216.34 \pm 0.02$	K	NIST Webbook
$T_{\text{fus}}$	$216.34 \pm 0.02$	K	NIST Webbook
$T_{\text{fus}}$	$216.35 \pm 0.01$	K	NIST Webbook
$T_{\text{fus}}$	$215.90 \pm 0.40$	K	NIST Webbook
$T_{\text{fus}}$	$227.31 \pm 0.20$	K	NIST Webbook
$T_{\text{fus}}$	$216.00 \pm 2.00$	K	NIST Webbook

Property	Value	Unit	Source
$T_{\text{fus}}$	$216.15 \pm 1.50$	K	NIST Webbook
$T_{\text{fus}}$	$216.15 \pm 0.50$	K	NIST Webbook
$T_{\text{fus}}$	$216.31 \pm 0.05$	K	NIST Webbook
$T_{\text{fus}}$	$216.25 \pm 0.30$	K	NIST Webbook
$T_{\text{fus}}$	$216.35 \pm 0.40$	K	NIST Webbook
$T_{\text{fus}}$	$216.65 \pm 0.30$	K	NIST Webbook
$T_{\text{fus}}$	$216.35 \pm 0.20$	K	NIST Webbook
$T_{\text{fus}}$	$217.15 \pm 2.00$	K	NIST Webbook
$T_{\text{fus}}$	$216.00 \pm 2.00$	K	NIST Webbook
$T_{\text{fus}}$	$216.33 \pm 0.10$	K	NIST Webbook
$T_{\text{fus}}$	$216.25 \pm 0.50$	K	NIST Webbook
$T_{\text{fus}}$	$216.25 \pm 0.08$	K	NIST Webbook
$T_{\text{fus}}$	$216.65 \pm 0.30$	K	NIST Webbook
$T_{\text{triple}}$	$216.37 \pm 0.40$	K	NIST Webbook
$T_{\text{triple}}$	$216.37 \pm 0.03$	K	NIST Webbook
$T_{\text{triple}}$	$216.36 \pm 0.20$	K	NIST Webbook
$T_{\text{triple}}$	$216.37 \pm 0.20$	K	NIST Webbook
$T_{\text{triple}}$	$216.36 \pm 0.05$	K	NIST Webbook
$T_{\text{triple}}$	$216.37 \pm 0.02$	K	NIST Webbook
$T_{\text{triple}}$	$215.80 \pm 0.20$	K	NIST Webbook
$T_{\text{triple}}$	$215.85 \pm 0.20$	K	NIST Webbook
$T_{\text{triple}}$	$215.60 \pm 0.25$	K	NIST Webbook
$V_c$	0.492	$\text{m}^3/\text{kg}\cdot\text{mol}$	NIST Webbook

## Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,\text{gas}}$	$232.74 \pm 0.47$	J/mol $\times$ K	385.65	NIST Webbook



Property	Value	Unit	Temperature (K)	Source
$C_{p,gas}$	238.95 ± 0.48	J/mol×K	398.15	NIST Webbook
$C_{p,gas}$	242.67	J/mol×K	405.7	NIST Webbook
$C_{p,gas}$	250.59 ± 0.50	J/mol×K	423.15	NIST Webbook
$C_{p,gas}$	263.02 ± 0.53	J/mol×K	448.15	NIST Webbook
$C_{p,gas}$	270.70	J/mol×K	462.5	NIST Webbook
$C_{p,gas}$	274.84 ± 0.55	J/mol×K	473.15	NIST Webbook
$C_{p,gas}$	285.98 ± 0.57	J/mol×K	498.15	NIST Webbook
$C_{p,gas}$	295.39	J/mol×K	522.7	NIST Webbook
$C_{p,gas}$	297.00 ± 0.59	J/mol×K	523.15	NIST Webbook
$C_{p,liquid}$	247.70	J/mol×K	293.7	NIST Webbook
$C_{p,liquid}$	252.40	J/mol×K	297.54	NIST Webbook
$C_{p,liquid}$	252.40	J/mol×K	298.0	NIST Webbook
$C_{p,liquid}$	253.20	J/mol×K	298.0	NIST Webbook
$C_{p,liquid}$	255.68	J/mol×K	298.15	NIST Webbook
$C_{p,liquid}$	255.68	J/mol×K	298.15	NIST Webbook
$C_{p,liquid}$	255.68	J/mol×K	298.15	NIST Webbook
$C_{p,liquid}$	254.11	J/mol×K	298.15	NIST Webbook
$C_{p,liquid}$	255.68	J/mol×K	298.15	NIST Webbook
$C_{p,liquid}$	254.18	J/mol×K	298.15	NIST Webbook
$C_{p,liquid}$	253.72	J/mol×K	298.15	NIST Webbook
$C_{p,liquid}$	254.02	J/mol×K	298.15	NIST Webbook
$C_{p,liquid}$	254.07	J/mol×K	298.15	NIST Webbook
$C_{p,liquid}$	252.92	J/mol×K	298.15	NIST Webbook
$C_{p,liquid}$	254.14	J/mol×K	298.15	NIST Webbook
$C_{p,liquid}$	253.89	J/mol×K	298.15	NIST Webbook
$C_{p,liquid}$	251.50	J/mol×K	298.3	NIST Webbook
$C_{p,liquid}$	254.70	J/mol×K	299.0	NIST Webbook
$C_{p,liquid}$	253.93	J/mol×K	299.8	NIST Webbook

Property	Value	Unit	Temperature (K)	Source
$C_{p,liquid}$	262.20	J/mol×K	318.15	NIST Webbook
$\eta$	0.0002448	Paxs	382.44	Joback Method
$\Delta_{fus} H$	20.09	kJ/mol	215.6	NIST Webbook
$\Delta_{fus} H$	20.65	kJ/mol	215.8	NIST Webbook
$\Delta_{fus} H$	20.74	kJ/mol	216.38	NIST Webbook
$\Delta_{fus} H$	20.74	kJ/mol	216.4	NIST Webbook
$\Delta_{fus} H$	21.80	kJ/mol	216.6	NIST Webbook
$\Delta_{sub} H$	68.10	kJ/mol	216.0	NIST Webbook
$\Delta_{vap} H$	44.40	kJ/mol	247.0	NIST Webbook
$\Delta_{vap} H$	43.00	kJ/mol	257.0	NIST Webbook
$\Delta_{vap} H$	38.00 ± 0.10	kJ/mol	311.0	NIST Webbook
$\Delta_{vap} H$	40.50 ± 0.10	kJ/mol	313.0	NIST Webbook
$\Delta_{vap} H$	41.90	kJ/mol	315.5	NIST Webbook
$\Delta_{vap} H$	36.70 ± 0.10	kJ/mol	328.0	NIST Webbook
$\Delta_{vap} H$	39.10 ± 0.10	kJ/mol	333.0	NIST Webbook
$\Delta_{vap} H$	35.40 ± 0.10	kJ/mol	344.0	NIST Webbook
$\Delta_{vap} H$	41.00	kJ/mol	348.5	NIST Webbook
$\Delta_{vap} H$	41.20	kJ/mol	348.5	NIST Webbook
$\Delta_{vap} H$	37.80 ± 0.10	kJ/mol	353.0	NIST Webbook
$\Delta_{vap} H$	39.20	kJ/mol	363.0	NIST Webbook
$\Delta_{vap} H$	34.41	kJ/mol	398.8	NIST Webbook
$\Delta_{vap} H$	36.30	kJ/mol	414.0	NIST Webbook
$\Delta_{vap} H$	39.40	kJ/mol	443.0	NIST Webbook
$\Delta_{vap} H$	35.50	kJ/mol	469.0	NIST Webbook
$\Delta_{vap} H$	34.90	kJ/mol	537.5	NIST Webbook
$\Delta_{fus} S$	93.19	J/mol×K	215.6	NIST Webbook
$\Delta_{fus} S$	95.70	J/mol×K	215.8	NIST Webbook
$\Delta_{fus} S$	95.85	J/mol×K	216.38	NIST Webbook

## Sources

**Joback Method:** [https://en.wikipedia.org/wiki/Joback\\_method](https://en.wikipedia.org/wiki/Joback_method)

**NIST Webbook:** <http://webbook.nist.gov/cgi/inchi/InChI=1S/C8H18/c1-3-5-7-8-6-4-2/h3-8H2,1-2H3>

**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

## Legend

$\Delta_c H^\circ_{\text{liquid}}$ : Standard liquid enthalpy of combustion (kJ/mol).

$C_{p,\text{gas}}$ : Ideal gas heat capacity (J/mol×K).

$C_{p,\text{liquid}}$ : Liquid phase heat capacity (J/mol×K).

$\eta$ : Dynamic viscosity (Pa×s).

$\Delta_f G^\circ$ : Standard Gibbs free energy of formation (kJ/mol).

$\Delta_f H^\circ_{\text{gas}}$ : Enthalpy of formation at standard conditions (kJ/mol).

$\Delta_f H^\circ_{\text{liquid}}$ : Liquid phase enthalpy of formation at standard conditions (kJ/mol).

$\Delta_{\text{fus}} H^\circ$ : Enthalpy of fusion at standard conditions (kJ/mol).

$\Delta_{\text{fus}} H$ : Enthalpy of fusion at a given temperature (kJ/mol).

$\Delta_{\text{sub}} H$ : Enthalpy of sublimation at a given temperature (kJ/mol).

$\Delta_{\text{vap}} H^\circ$ : Enthalpy of vaporization at standard conditions (kJ/mol).

$\Delta_{\text{vap}} H$ : Enthalpy of vaporization at a given temperature (kJ/mol).

**IE**: Ionization energy (eV).

**logP<sub>oct/wat</sub>**: Octanol/Water partition coefficient .

**P<sub>c</sub>**: Critical Pressure (kPa).

$\Delta_{\text{fus}} S$ : Entropy of fusion at a given temperature (J/mol×K).

**S<sup>o</sup><sub>gas</sub>**: Molar entropy at standard conditions (J/mol×K).

**S<sup>o</sup><sub>liquid</sub>**: Liquid phase molar entropy at standard conditions (J/mol×K).

**T<sub>boil</sub>**: Normal Boiling Point Temperature (K).

**T<sub>c</sub>**: Critical Temperature (K).

**T<sub>fus</sub>**: Normal melting (fusion) point (K).

**T<sub>triple</sub>**: Triple Point Temperature (K).

**V<sub>c</sub>**: Critical Volume (m<sup>3</sup>/kg-mol).

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