

2-Octenal, (E)-

Other names:	(E)-2-Octen-1-al
	(E)-2-Octenal
	(E)-Oct-2-enal
	2-(E)-Octenal
	Oct-(E)-2-enal
	Oct-2(E)-enal
	trans-2-Octen-1-al
	trans-2-Octenal
	trans-Oct-2-enal
Inchi:	InChI=1S/C8H14O/c1-2-3-4-5-6-7-8-9/h6-8H,2-5H2,1H3/b7-6+
InchiKey:	LVBXEMGDVWVTGY-VOTSOKGWSA-N
Formula:	C8H14O
SMILES:	CCCCC=CC=O
Mol. weight [g/mol]:	126.20
CAS:	2548-87-0

Physical Properties

Property code	Value	Unit	Source
gf	-2.82	kJ/mol	Joback Method
hf	-176.81	kJ/mol	Joback Method
hfus	18.97	kJ/mol	Joback Method
hvap	40.08	kJ/mol	Joback Method
log10ws	-2.30		Crippen Method
logp	2.322		Crippen Method
mcvol	120.850	ml/mol	McGowan Method
pc	2890.51	kPa	Joback Method
rinpol	1045.00		NIST Webbook
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ripol	1425.00		NIST Webbook
ripol	1422.00		NIST Webbook
ripol	1421.00		NIST Webbook
tb	435.26	K	Joback Method
tc	614.34	K	Joback Method
tf	216.84	K	Joback Method
vc	0.480	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	241.07	J/molxK	435.26	Joback Method
cpg	295.10	J/molxK	584.49	Joback Method
cpg	285.31	J/molxK	554.65	Joback Method
cpg	275.03	J/molxK	524.80	Joback Method
cpg	264.25	J/molxK	494.95	Joback Method
cpg	252.93	J/molxK	465.11	Joback Method
cpg	304.43	J/molxK	614.34	Joback Method
dvisc	0.0002628	Paxs	435.26	Joback Method
dvisc	0.0003402	Paxs	398.86	Joback Method
dvisc	0.0004641	Paxs	362.45	Joback Method
dvisc	0.0006784	Paxs	326.05	Joback Method
dvisc	0.0010910	Paxs	289.65	Joback Method
dvisc	0.0020114	Paxs	253.24	Joback Method
dvisc	0.0045537	Paxs	216.84	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	358.20	K	2.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.51611e+01
Coeff. B	-4.09803e+03
Coeff. C	-6.87940e+01
Temperature range (K), min.	344.32
Temperature range (K), max.	484.85

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=C2548870&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure

pvap:	Vapor pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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