(Z)-2-octenal

Other names: 2-Octenal, (Z)-
2-(Z)-Octenal
(Z)-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-SREVYHEPSA-N
Formula: C8H14O
SMILES: CCCCCC=CC=O
Mol. weight [g/mol]: 126.20
CAS: 20664-46-4

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	1042.00		NIST Webbook
rinpol	1049.00		NIST Webbook
rinpol	1057.00		NIST Webbook
rinpol	1043.00		NIST Webbook
rinpol	1043.00		NIST Webbook
rinpol	1059.00		NIST Webbook
rinpol	1058.00		NIST Webbook
rinpol	1046.00		NIST Webbook
ripol	1413.00		NIST Webbook
ripol	1413.00		NIST Webbook
ripol	1413.00		NIST Webbook
ripol	1394.00		NIST Webbook
ripol	1379.00		NIST Webbook
ripol	1439.00		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/mol×K	435.26	Joback Method
cpg	252.93	J/mol×K	465.11	Joback Method
cpg	264.25	J/mol×K	494.95	Joback Method
cpg	275.03	J/mol×K	524.80	Joback Method
cpg	285.31	J/mol×K	554.65	Joback Method
cpg	295.10	J/mol×K	584.49	Joback Method
cpg	304.43	J/mol×K	614.34	Joback Method
dvisc	0.0045537	Pa×s	216.84	Joback Method
dvisc	0.0020114	Pa×s	253.24	Joback Method
dvisc	0.0010910	Pa×s	289.65	Joback Method
dvisc	0.0006784	Pa×s	326.05	Joback Method
dvisc	0.0004641	Pa×s	362.45	Joback Method
dvisc	0.0003402	Pa×s	398.86	Joback Method
dvisc	0.0002628	Pa×s	435.26	Joback Method

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C20664464&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
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume